

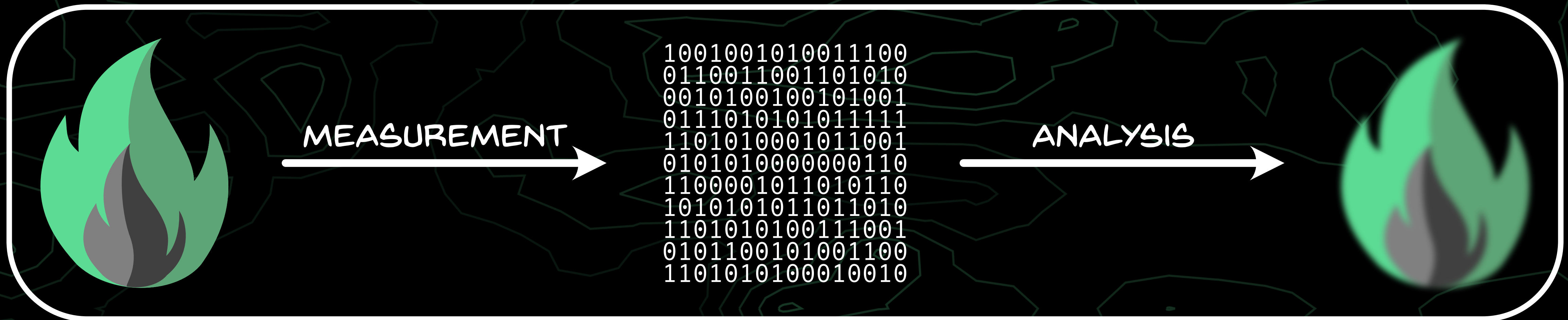
Accurate Estimation of Self- and Collective-Motion from Molecular Dynamics Simulation

PAQMAN — 2025-07-03



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scams-research.github.io
(he/him)

THE MEASUREMENT PROCESS IS A NOISY CHANNEL; INFORMATION IS LOST. THE ROLE OF ANALYSIS IS TO TRY AND RECONSTRUCT THE PHYSICAL OBSERVABLE.



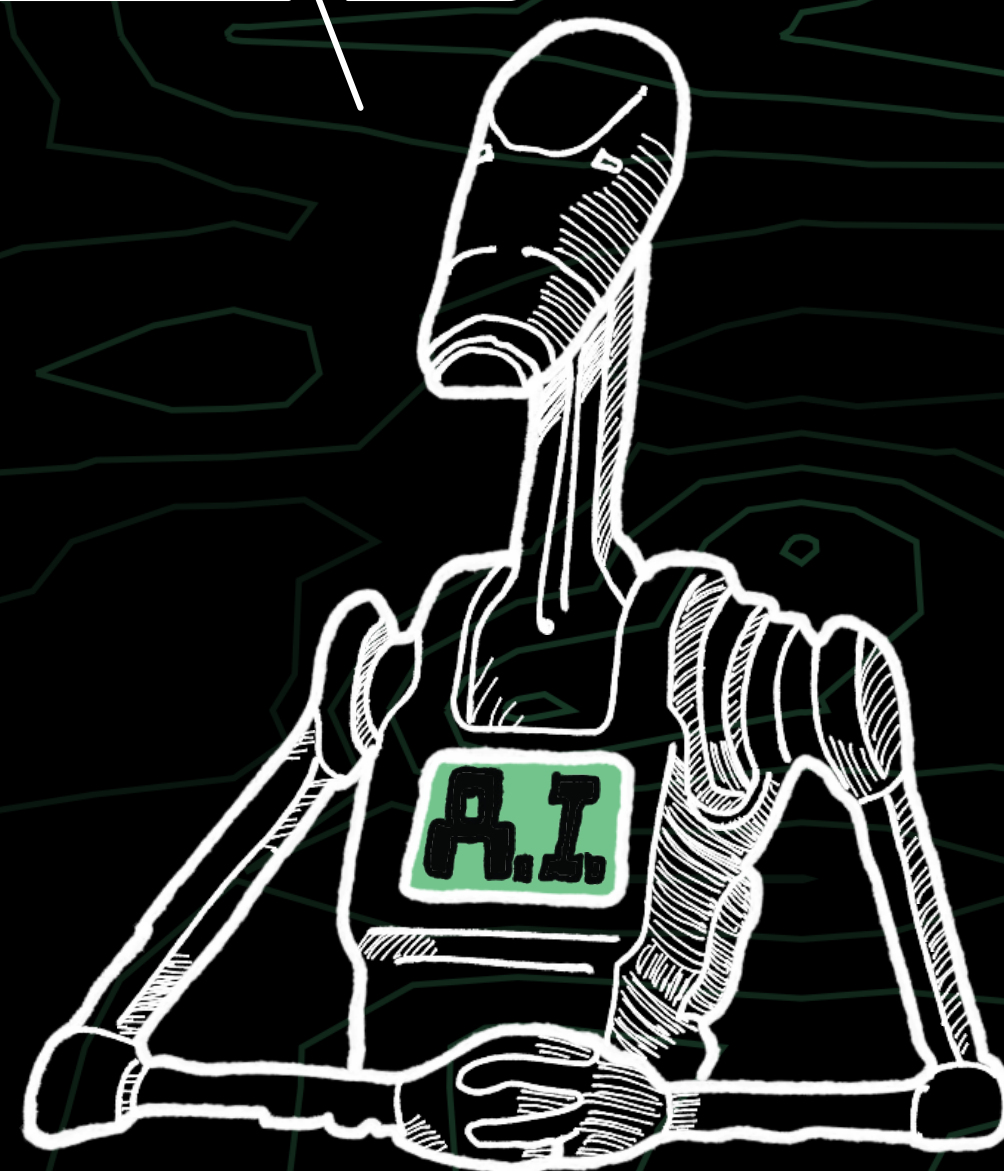
scams-research.github.io

DIFFUSION PLAYS AN IMPORTANT
ROLE IN ENERGY MATERIALS
AND INDUSTRIAL PROCESSES.



AN UNDERSTANDING OF
DIFFUSION CAN FACILITATE
RATIONAL DESIGN, LEVERAGING
ARTIFICIAL INTELLIGENCE.

ROGER ROGER.



PLUS, IT CAN BE FUN TO WORRY
ABOUT RANDOM WALKS.



ARRHENIUS MODELLING CAN
BE USED FOR DIFFUSION...

$\ln(D^*)$

x

x

x

x

T^{-1}

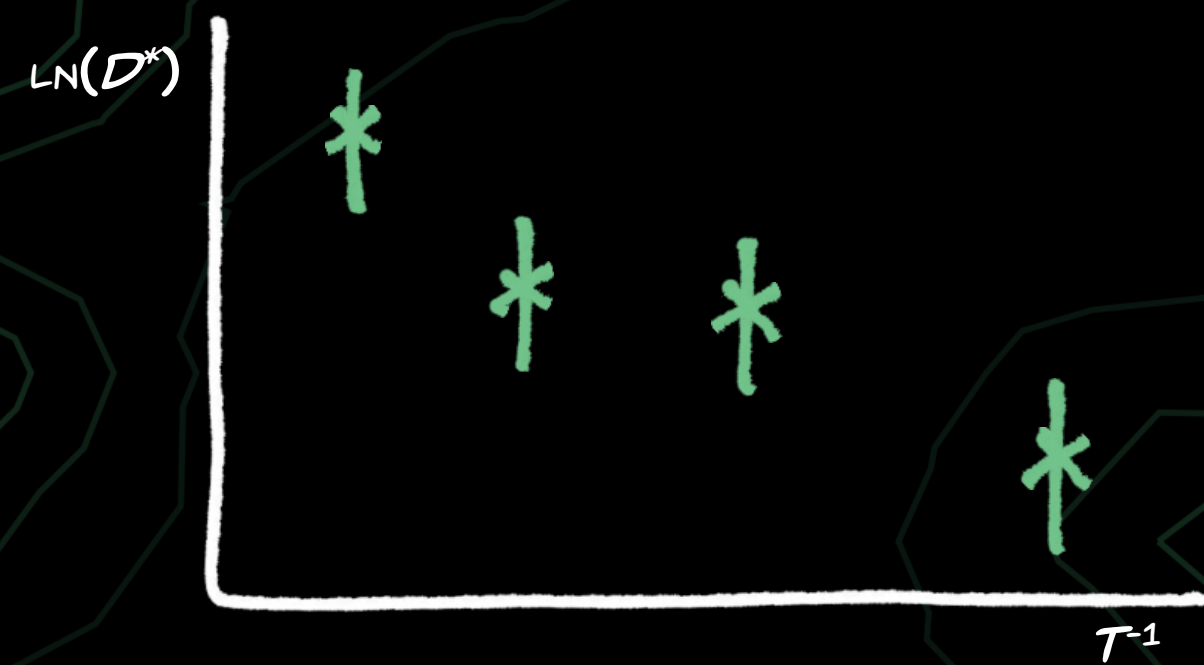


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ARRHENIUS MODELLING CAN
BE USED FOR DIFFUSION...



...AND WITHOUT ERROR BARS
RESULTS ARE MEANINGLESS.

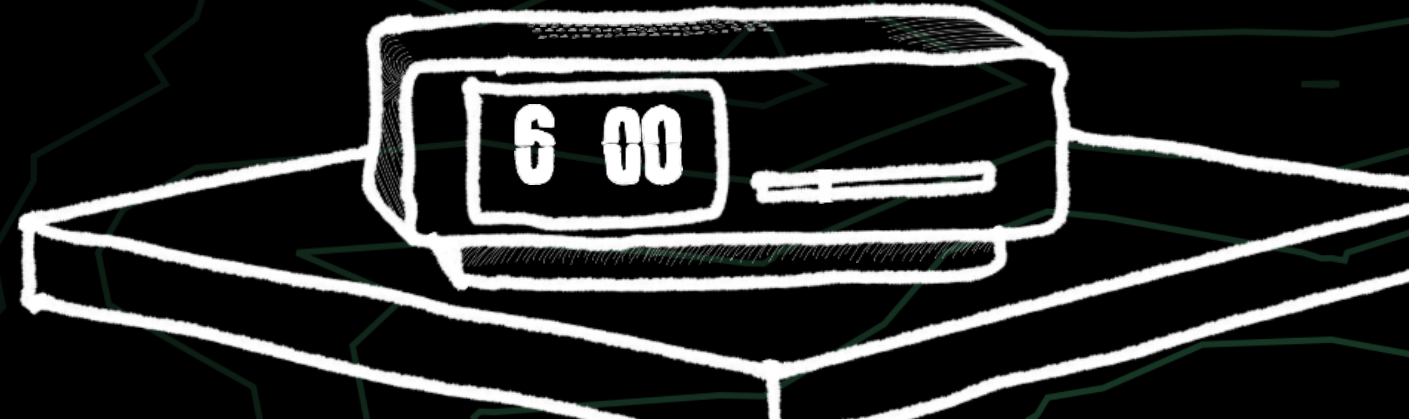


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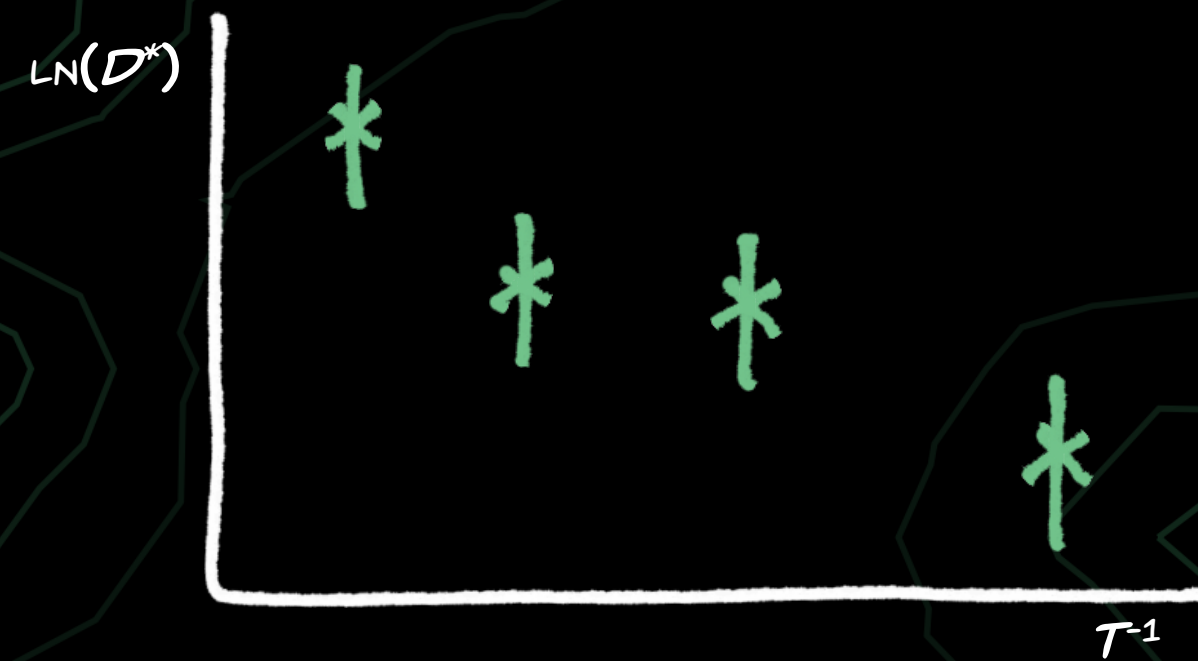


REPEATING SIMULATIONS CAN
BECOME TEDIOUS...

THEN PUT YOUR
LITTLE HAND IN MINE...



...AND WITHOUT ERROR BARS
RESULTS ARE MEANINGLESS.



THEN PUT YOUR
LITTLE HAND IN MINE...



THEN PUT YOUR
LITTLE HAND IN MINE...

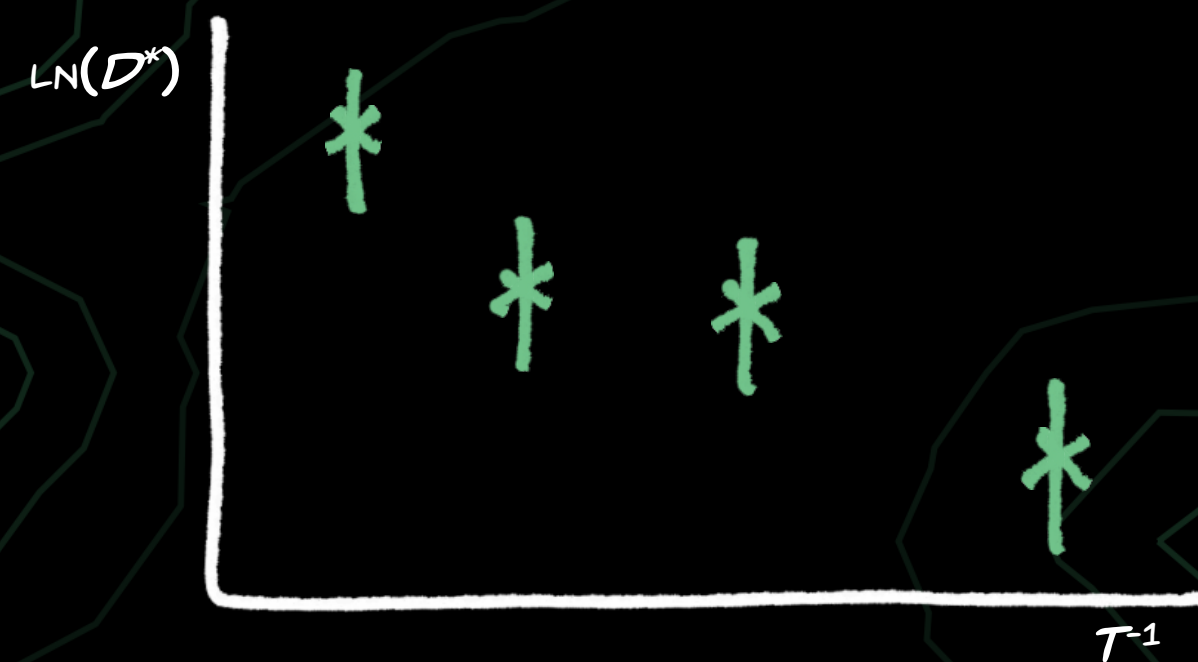


xN

ARRHENIUS MODELLING CAN
BE USED FOR DIFFUSION...

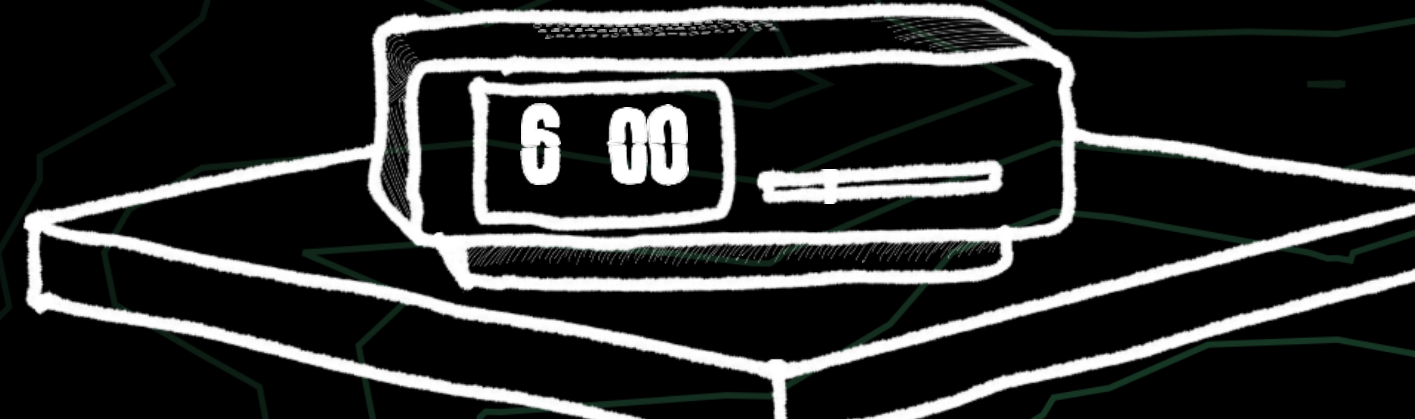


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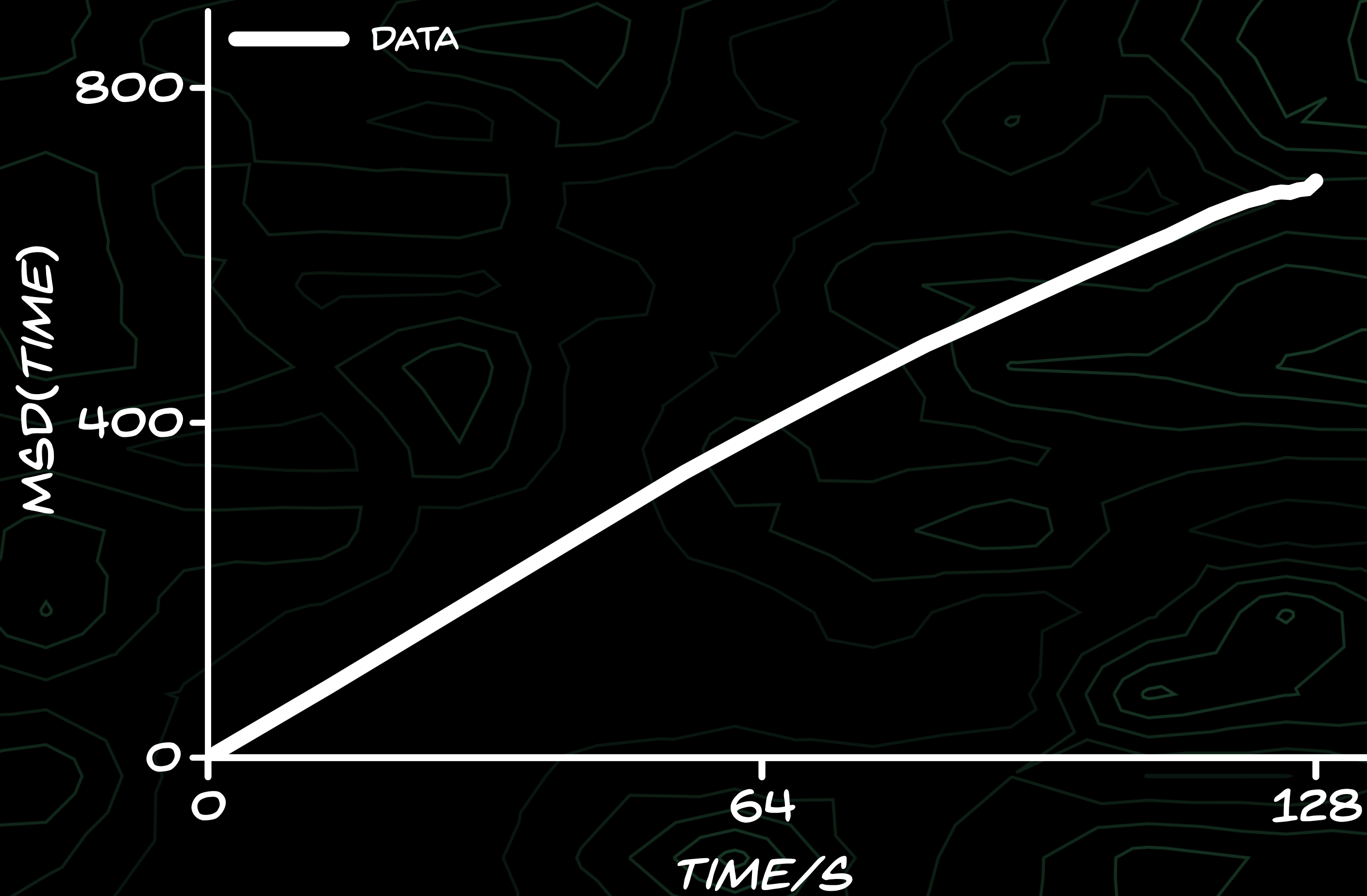
THEN PUT YOUR
LITTLE HAND IN MINE...

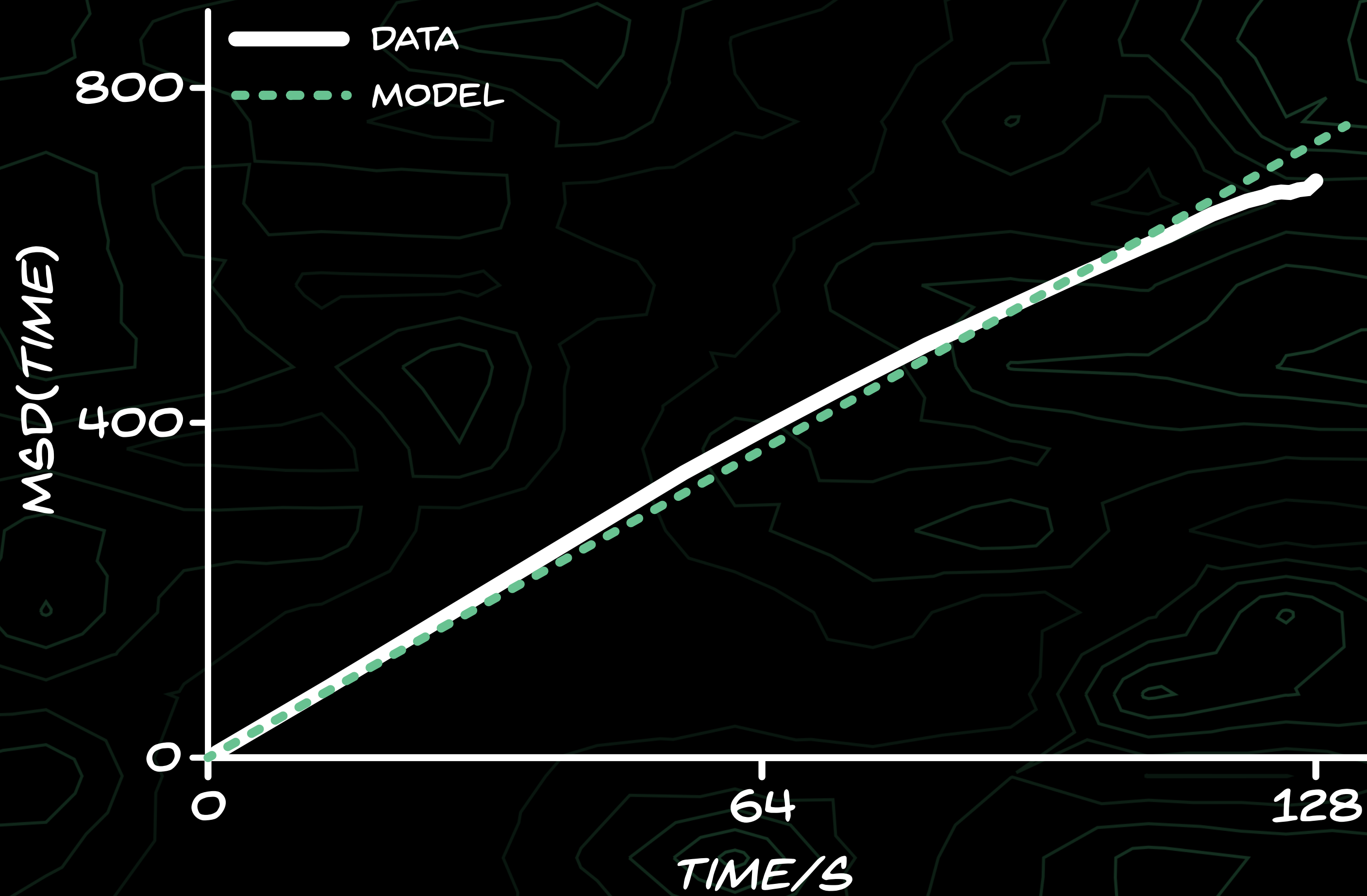


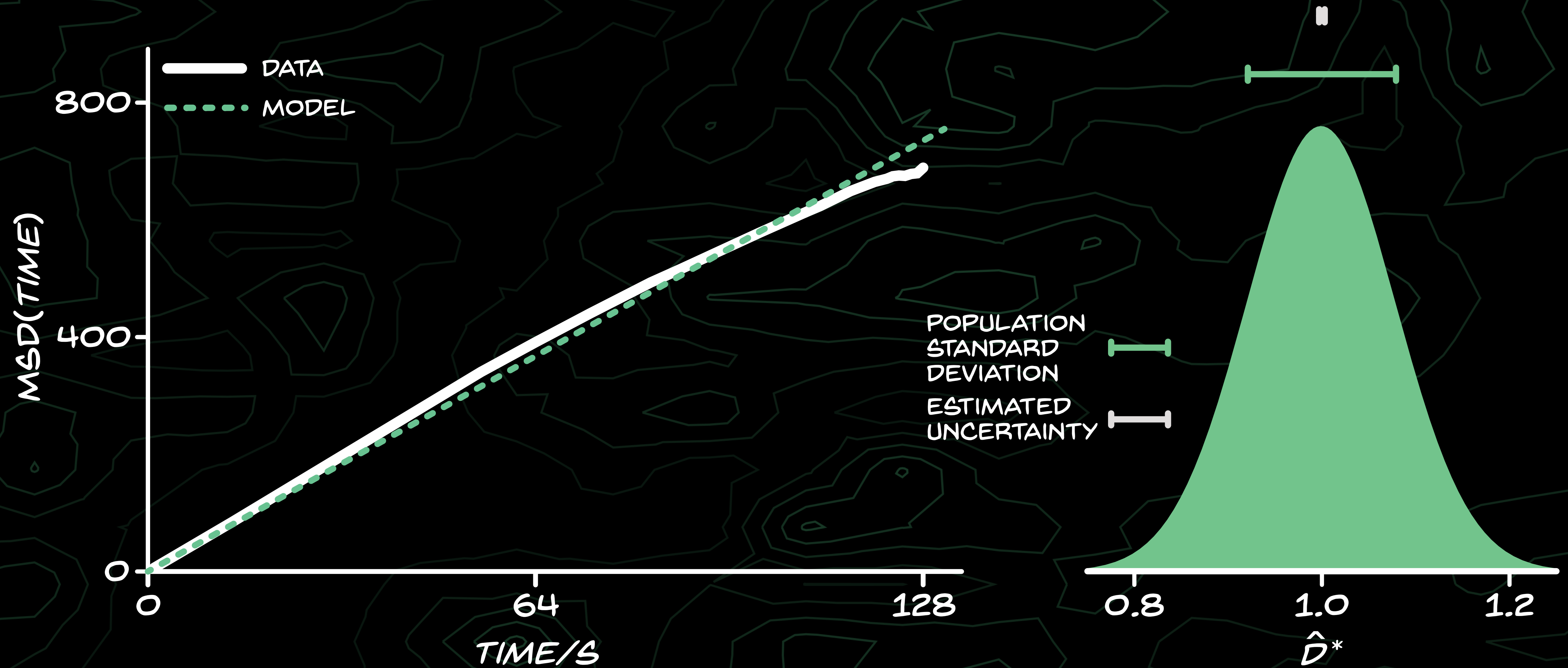
...SO WE WANT THE BEST WAY TO
MAXIMISE THE **PRECISION** OF
OUR ESTIMATE AND THE
ACCURACY OF THE VARIANCE
ESTIMATE.



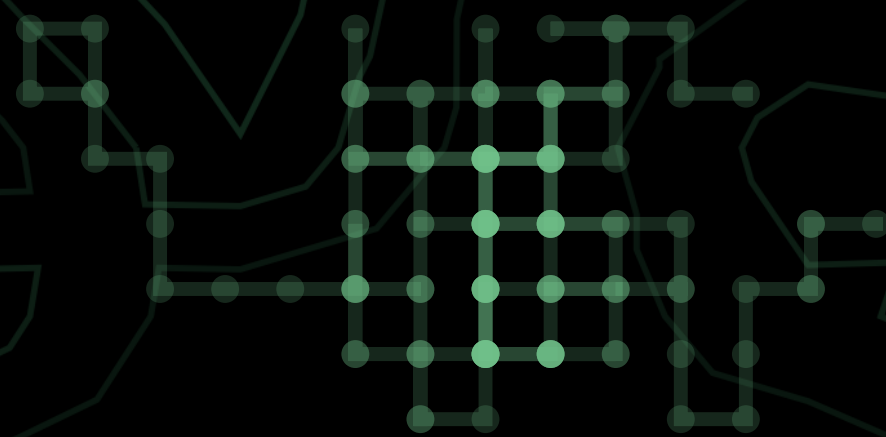
IDEALLY, FROM A SINGLE
MEASUREMENT.



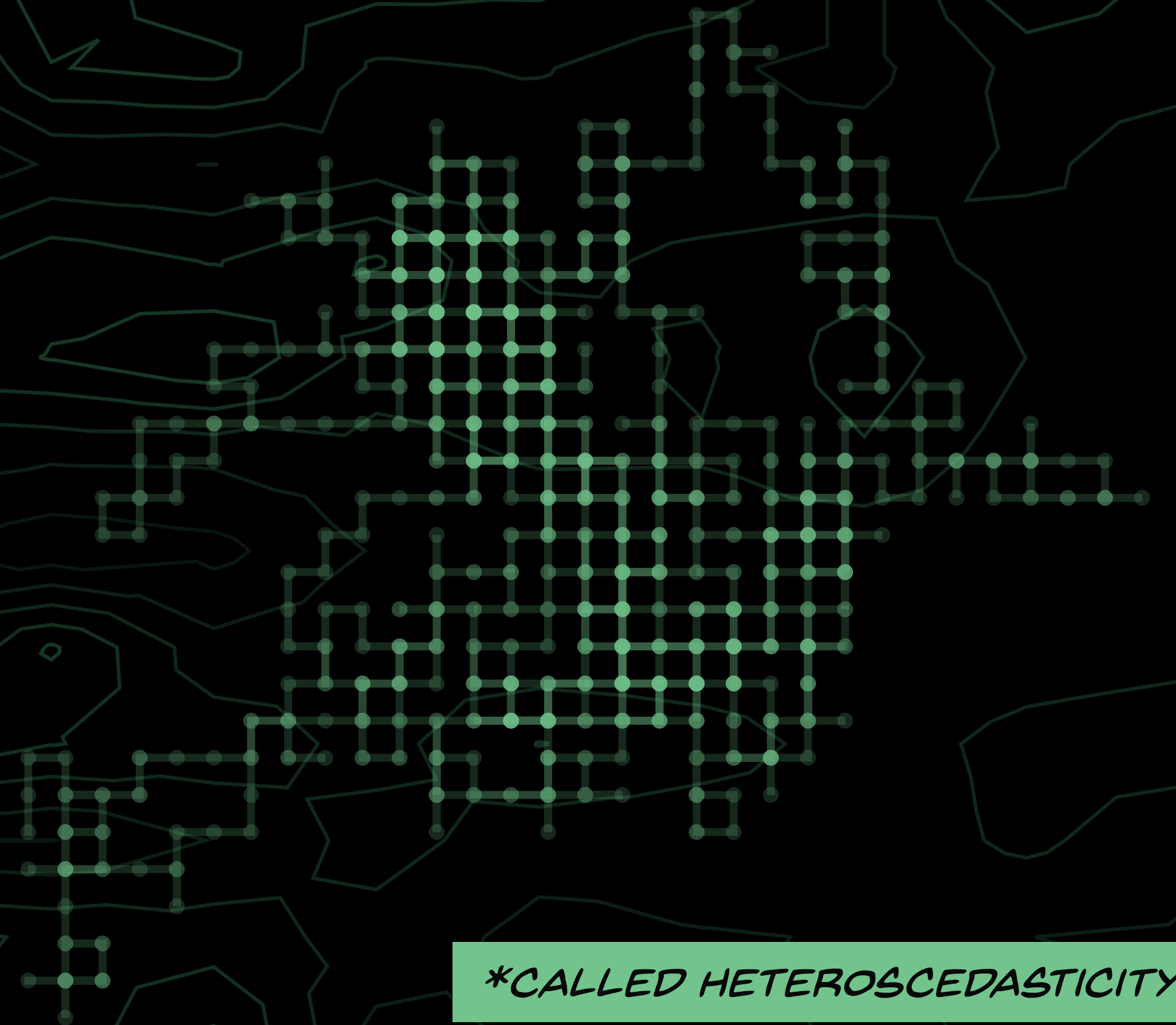




AFTER 16 2D RANDOM WALK STEPS, THERE ARE A RANGE OF VALUES OF DISPLACEMENT THAT CAN BE REACHED....

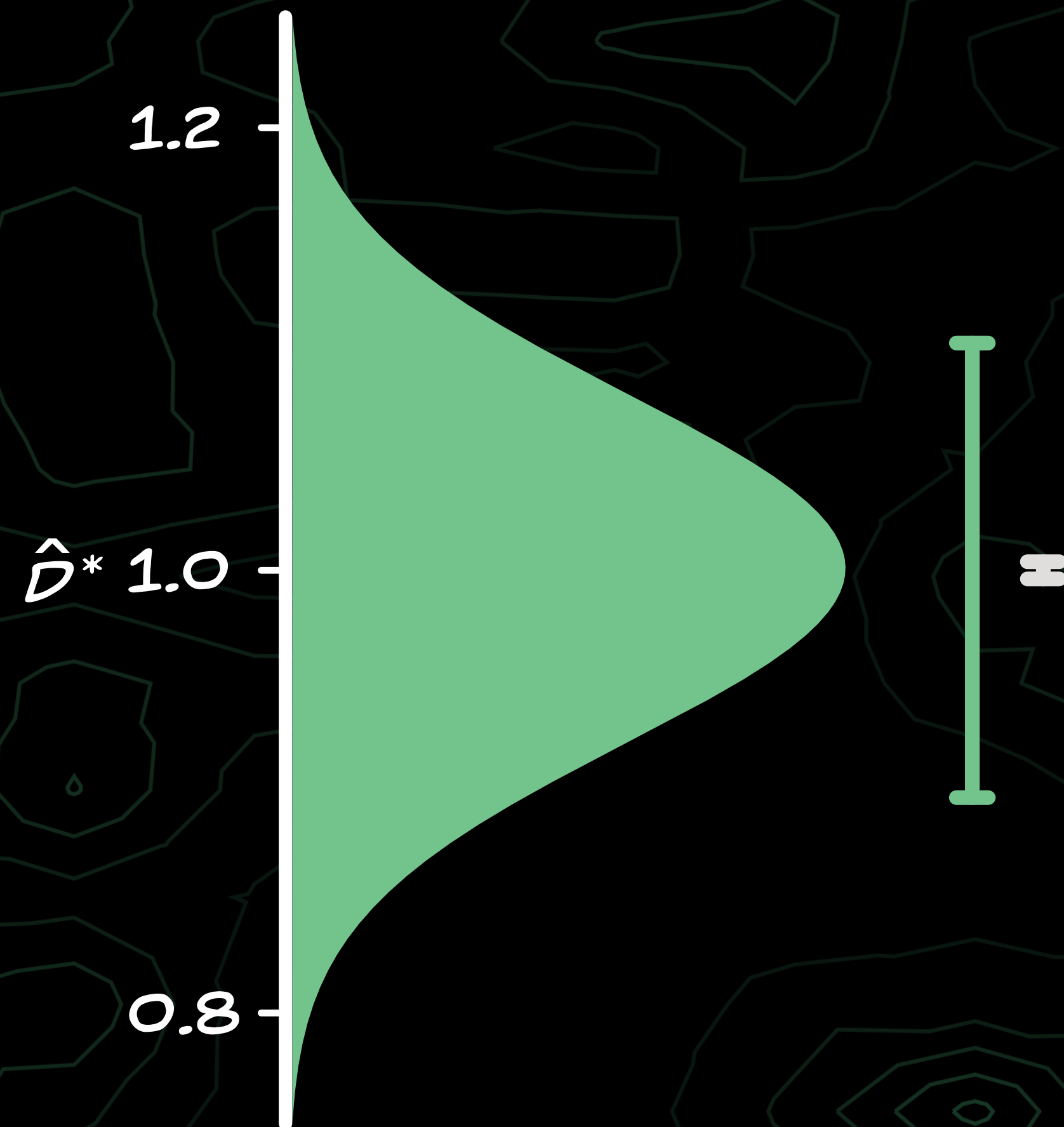


...AFTER LONGER PERIODS OF TIME, THAT RANGE (THE VARIANCE) INCREASES*.



*CALLED HETEROSCEDASTICITY

HOMOSCEDASTIC

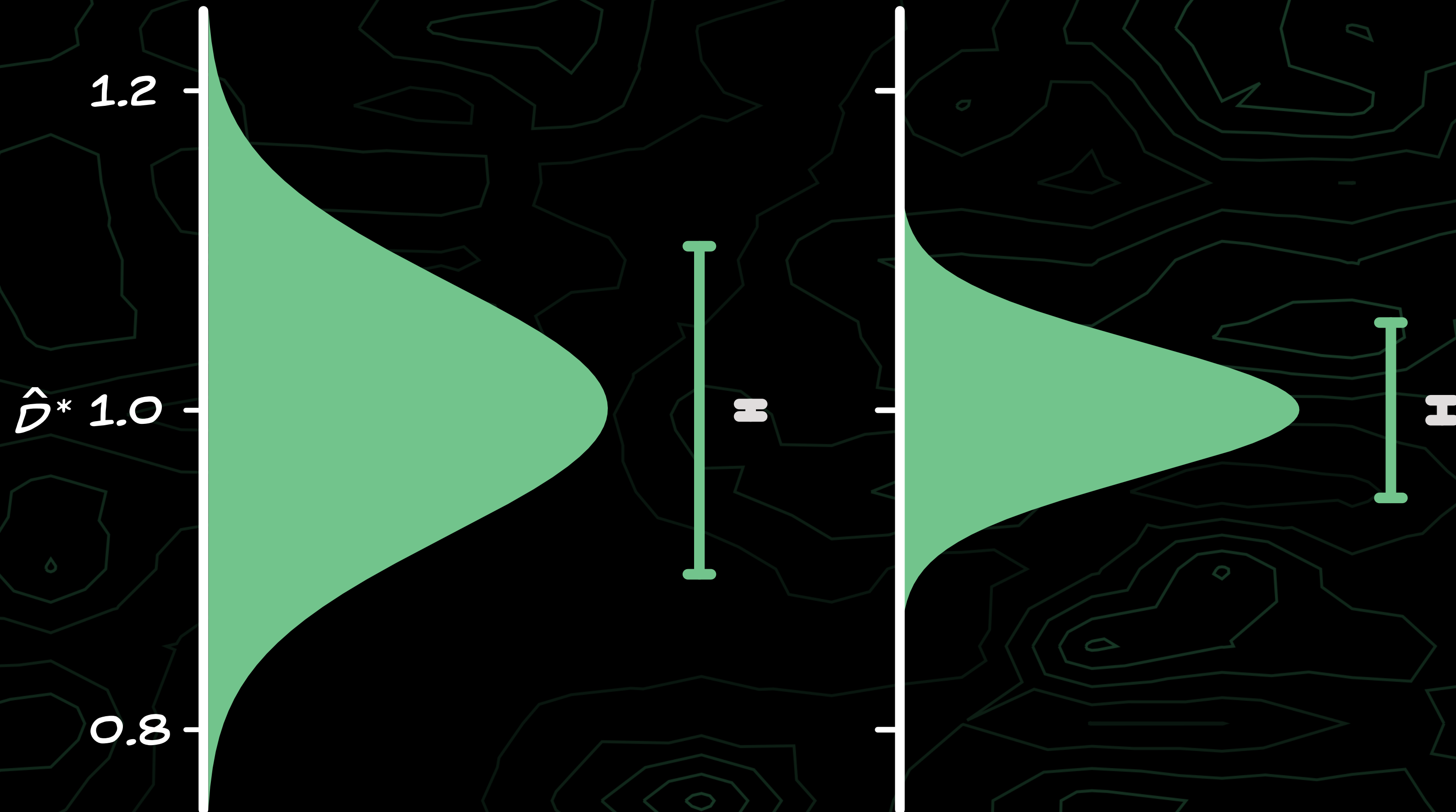


POPULATION STANDARD DEVIATION

ESTIMATED UNCERTAINTY

HOMOSCEDASTIC

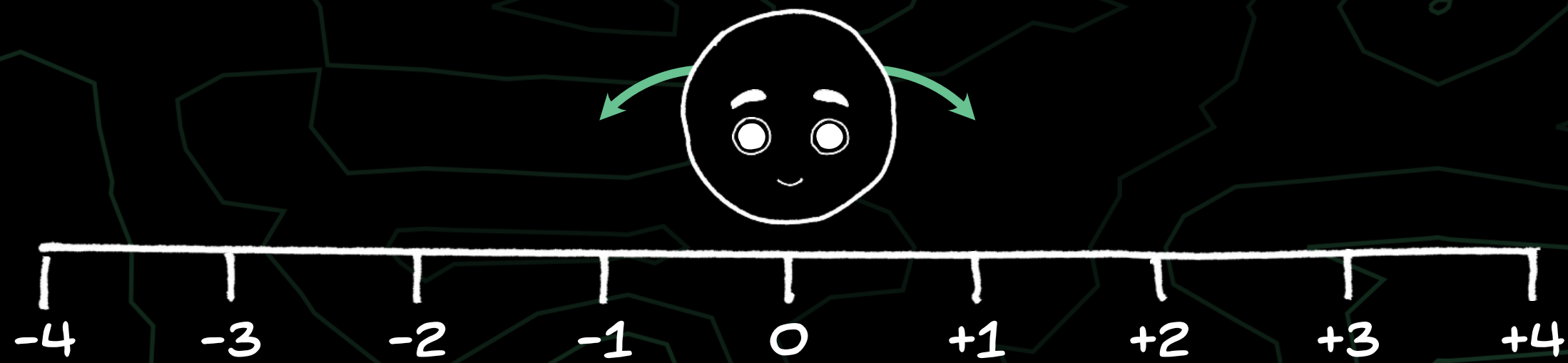
HETEROSCEDASTIC
AND UNCORRELATED



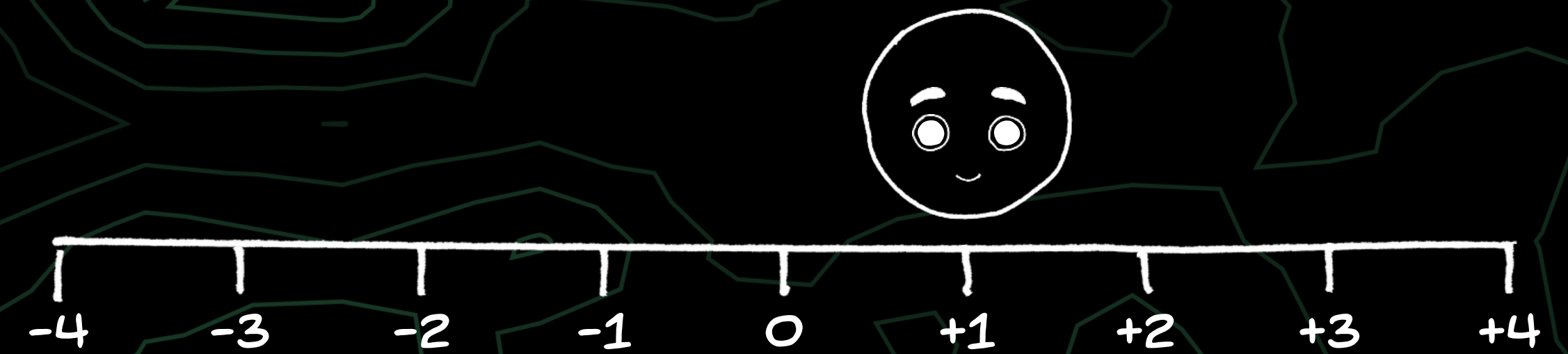
POPULATION STANDARD DEVIATION

ESTIMATED UNCERTAINTY

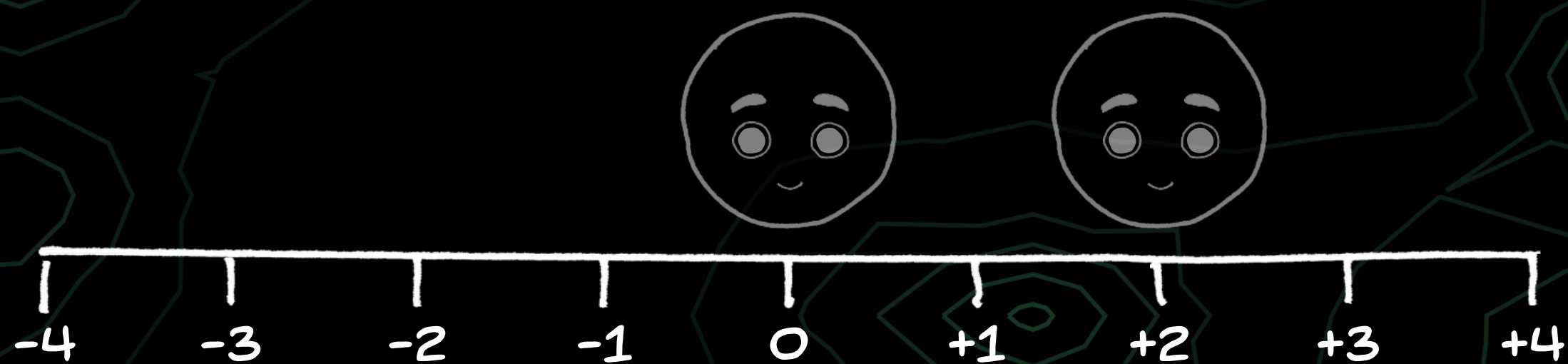
IF A PARTICLE ON A 1D RANDOM WALK WITH A STEP SIZE OF 1...



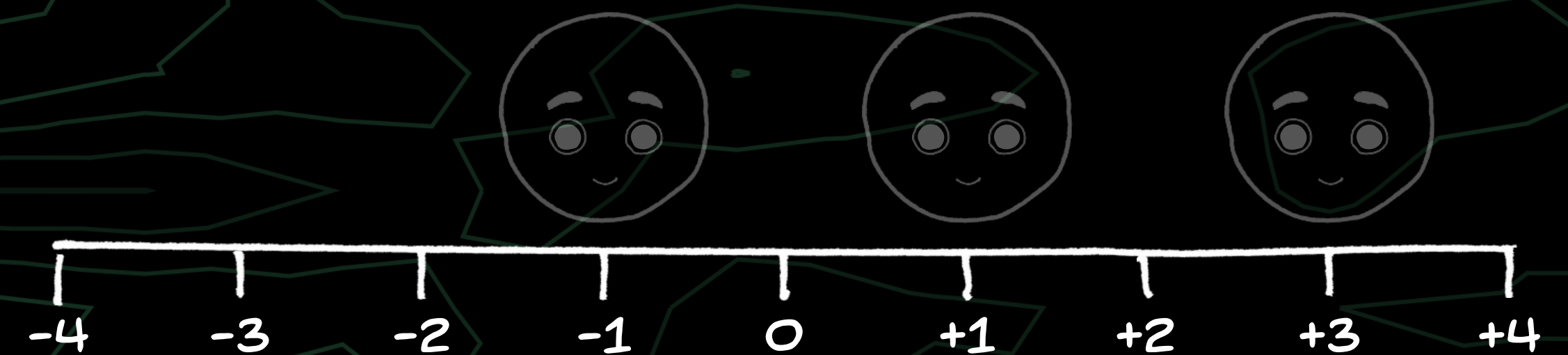
...AND AFTER 5 STEPS, IT GETS TO THE POSITION +1.



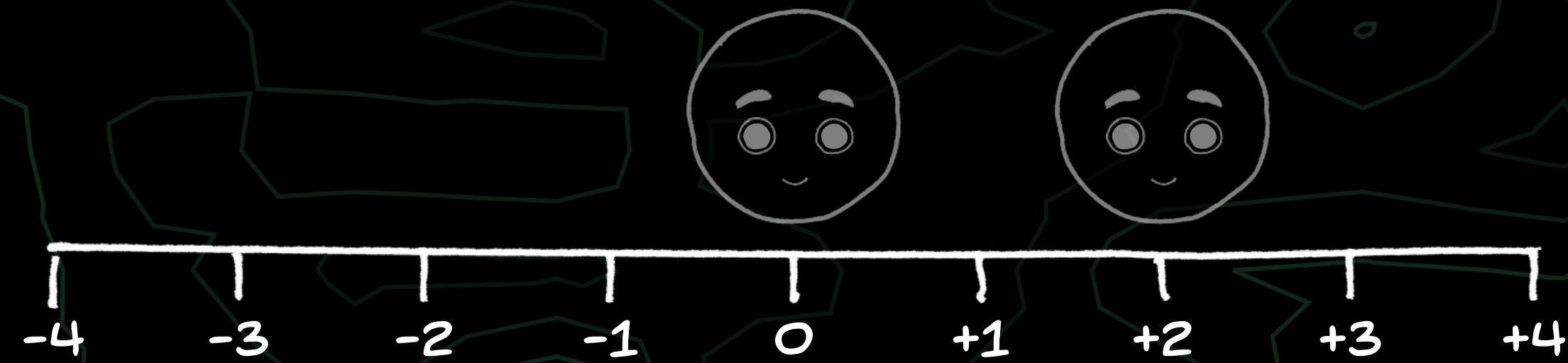
THEN AFTER 6 STEPS, IT COULD ONLY BE AT POSITIONS OF 0 OR +2...



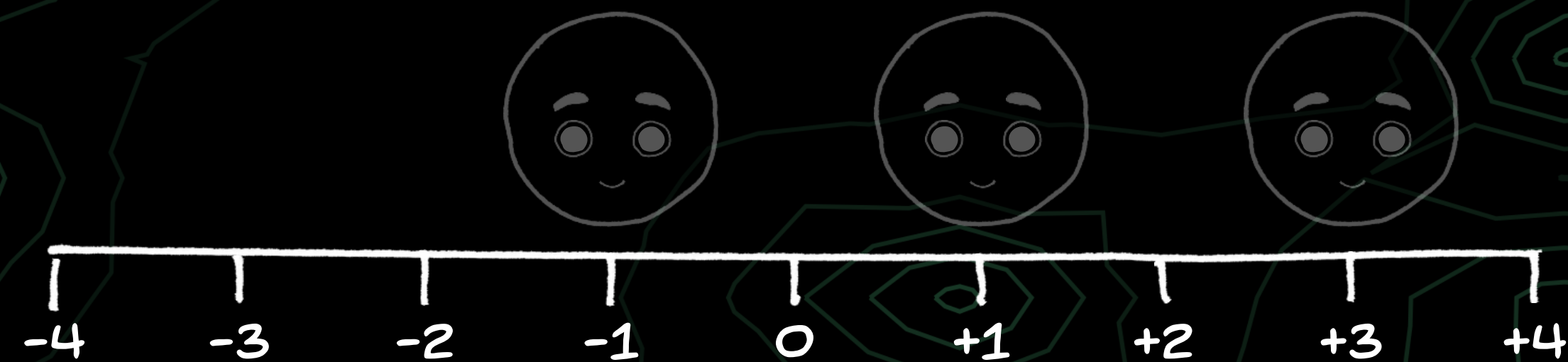
...AND AFTER 7 STEPS, IT CAN ONLY BE AT POSITIONS -1, +1, OR +3.



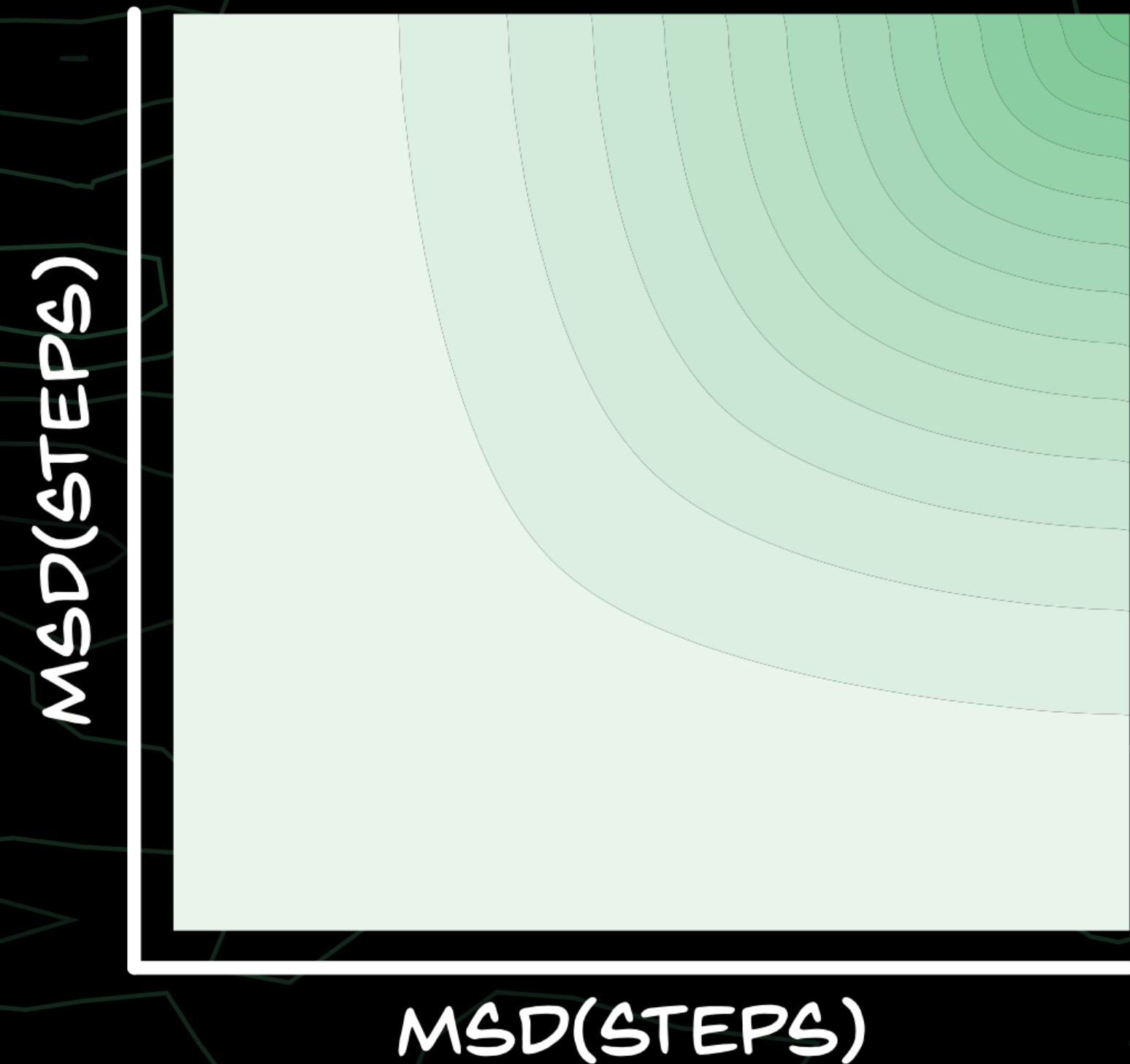
THEN AFTER 6 STEPS, IT COULD ONLY BE AT POSITIONS OF 0 OR +2...



...AND AFTER 7 STEPS, IT CAN ONLY BE AT POSITIONS -1, +1, OR +3.



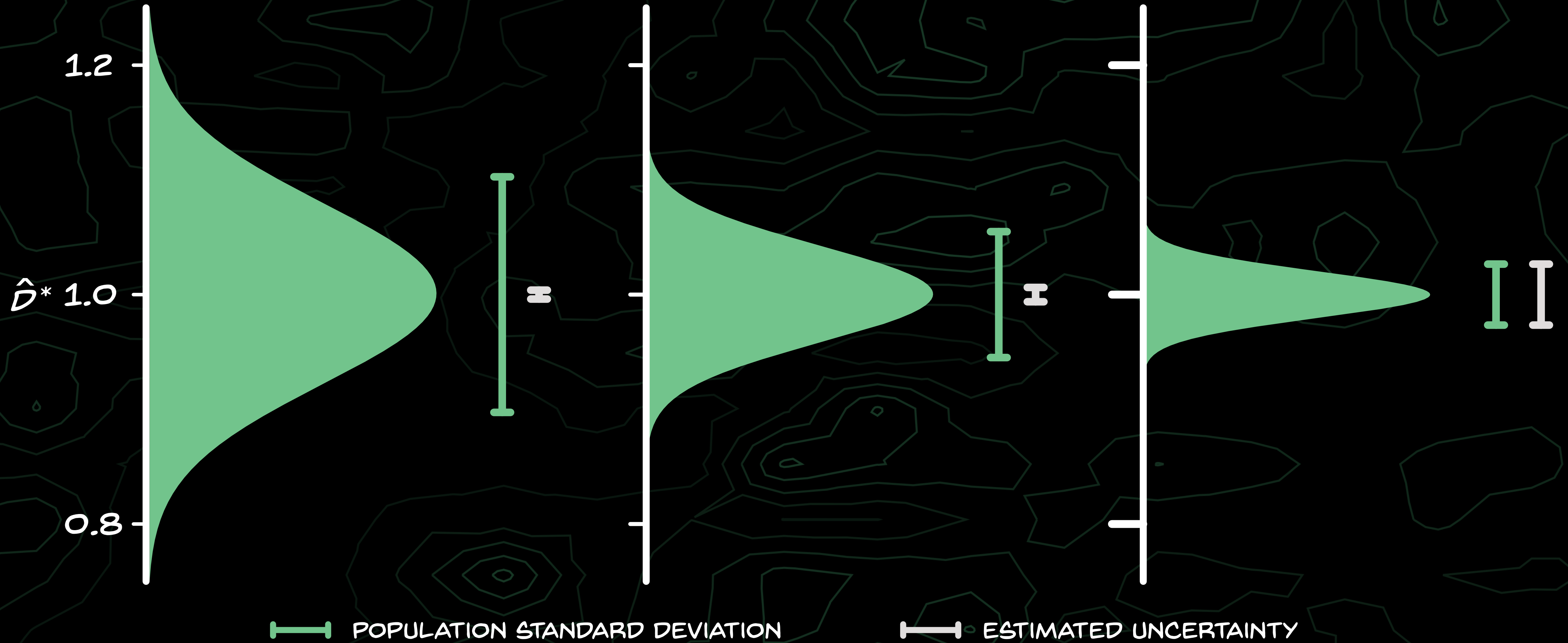
THE AMOUNT THAT THE DIFFERENT TIME POINTS INFLUENCE EACH OTHER IS DEFINED IN THE COVARIANCE MATRIX.



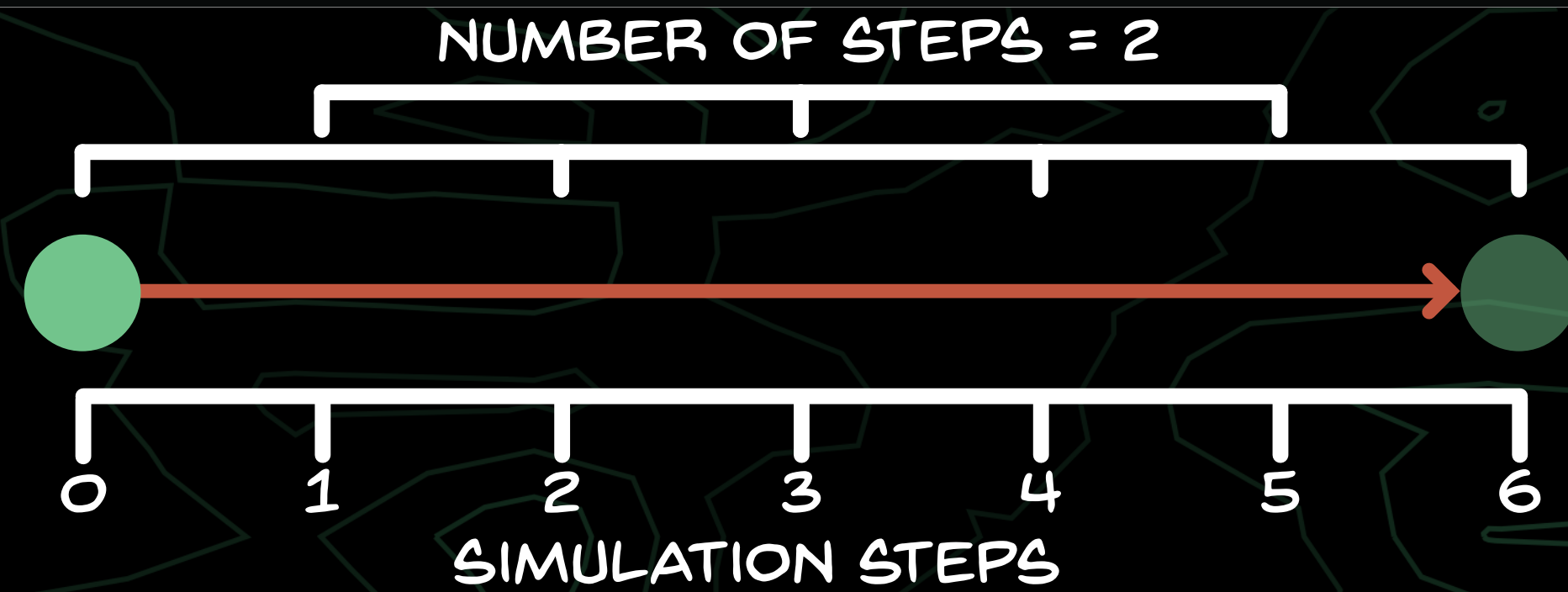
HOMOSCEDASTIC

HETEROSCEDASTIC
AND UNCORRELATED

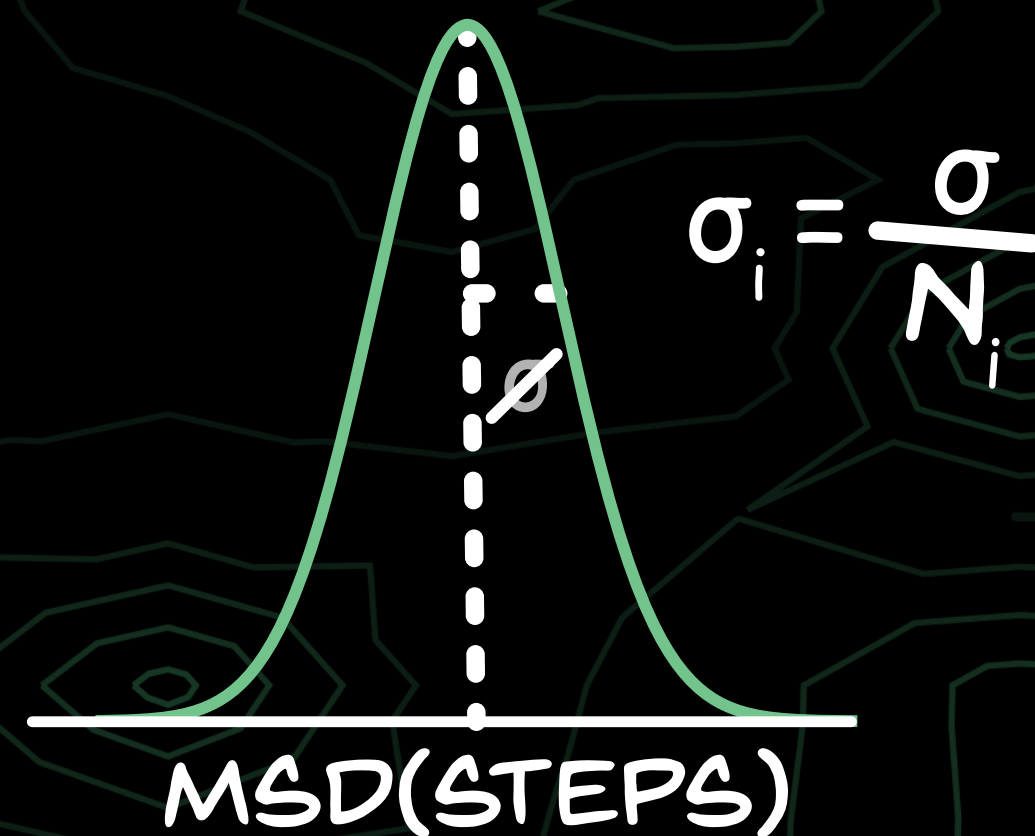
HETEROSCEDASTIC
AND CORRELATED



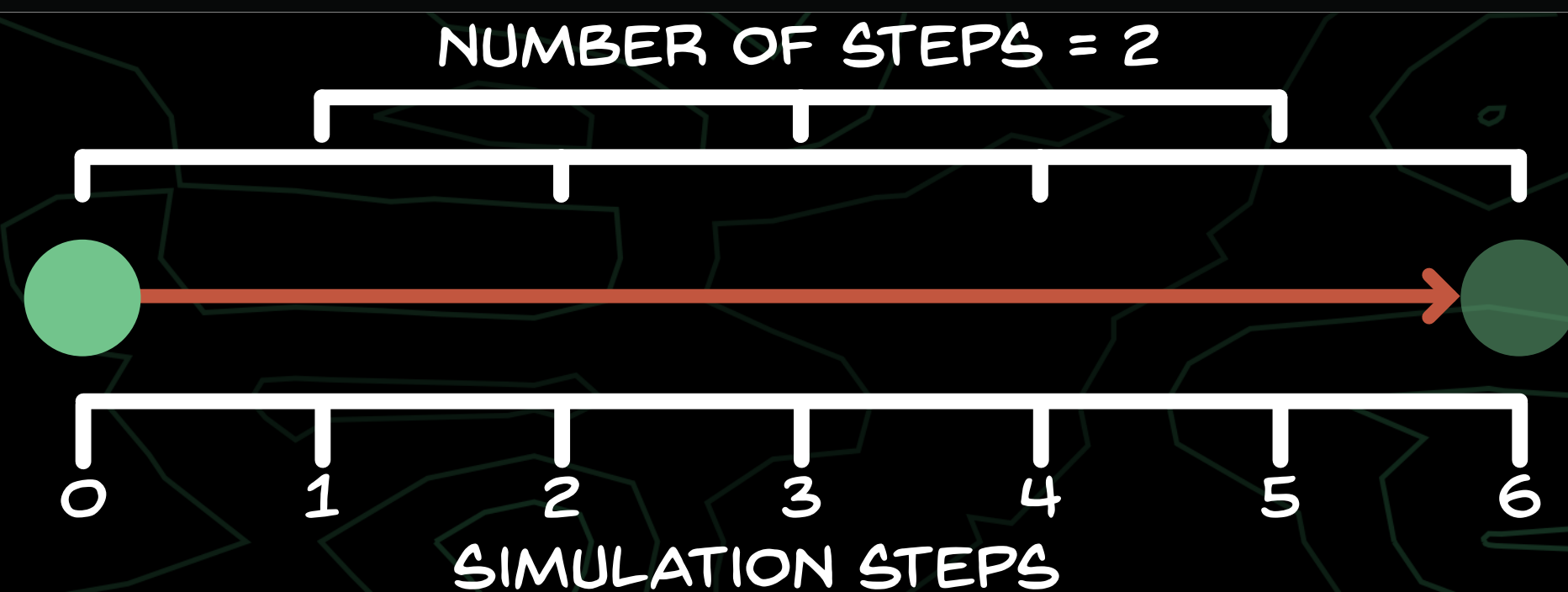
OVERLAPPING SAMPLES CAN MAXIMISE THE NUMBER OF OBSERVATIONS...



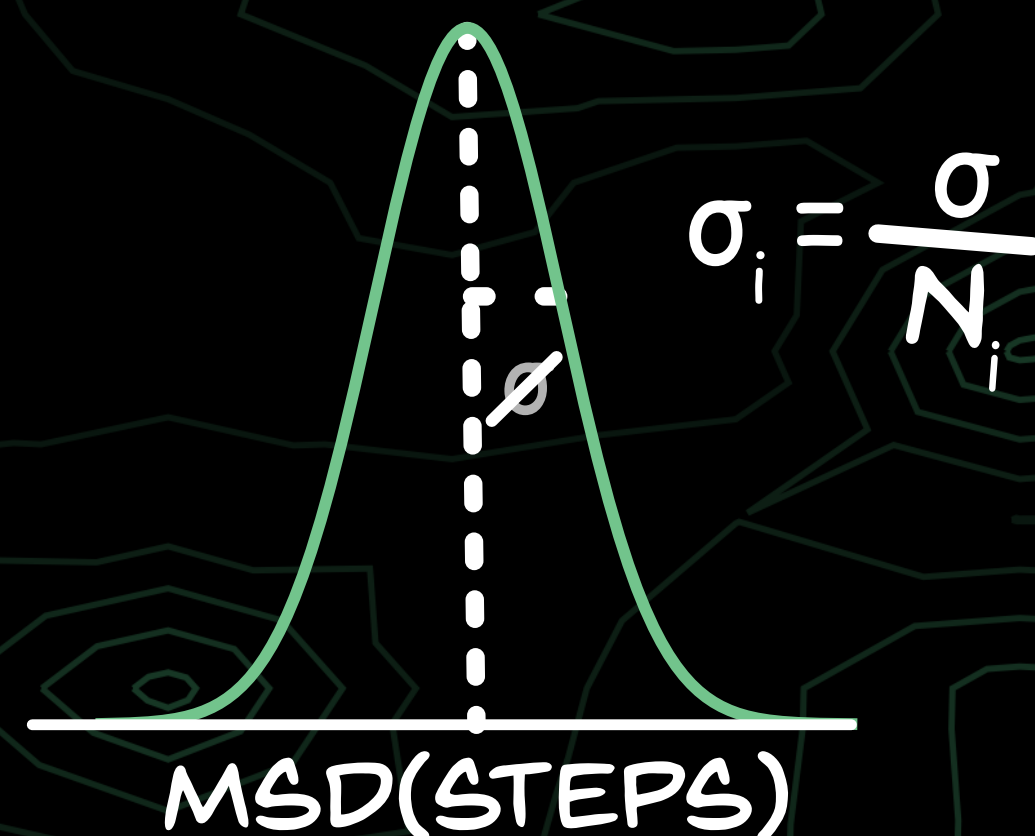
...HOWEVER, AS THE SAMPLES ARE **NOT** STATISTICALLY INDEPENDENT, THE VARIANCE MUST BE RESCALED BY THE NUMBER OF INDEPENDENT SAMPLES.



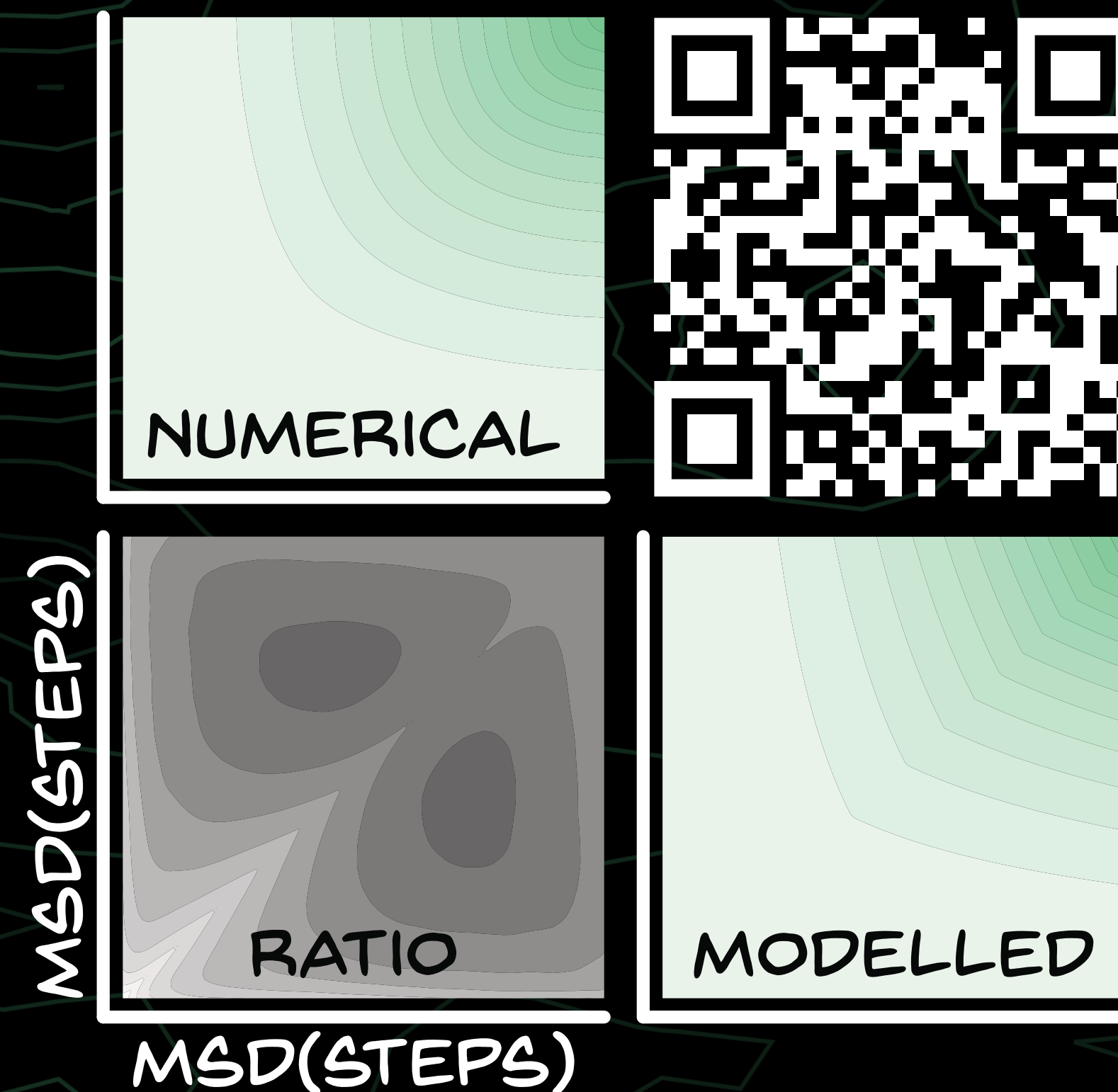
OVERLAPPING SAMPLES CAN MAXIMISE THE NUMBER OF OBSERVATIONS...

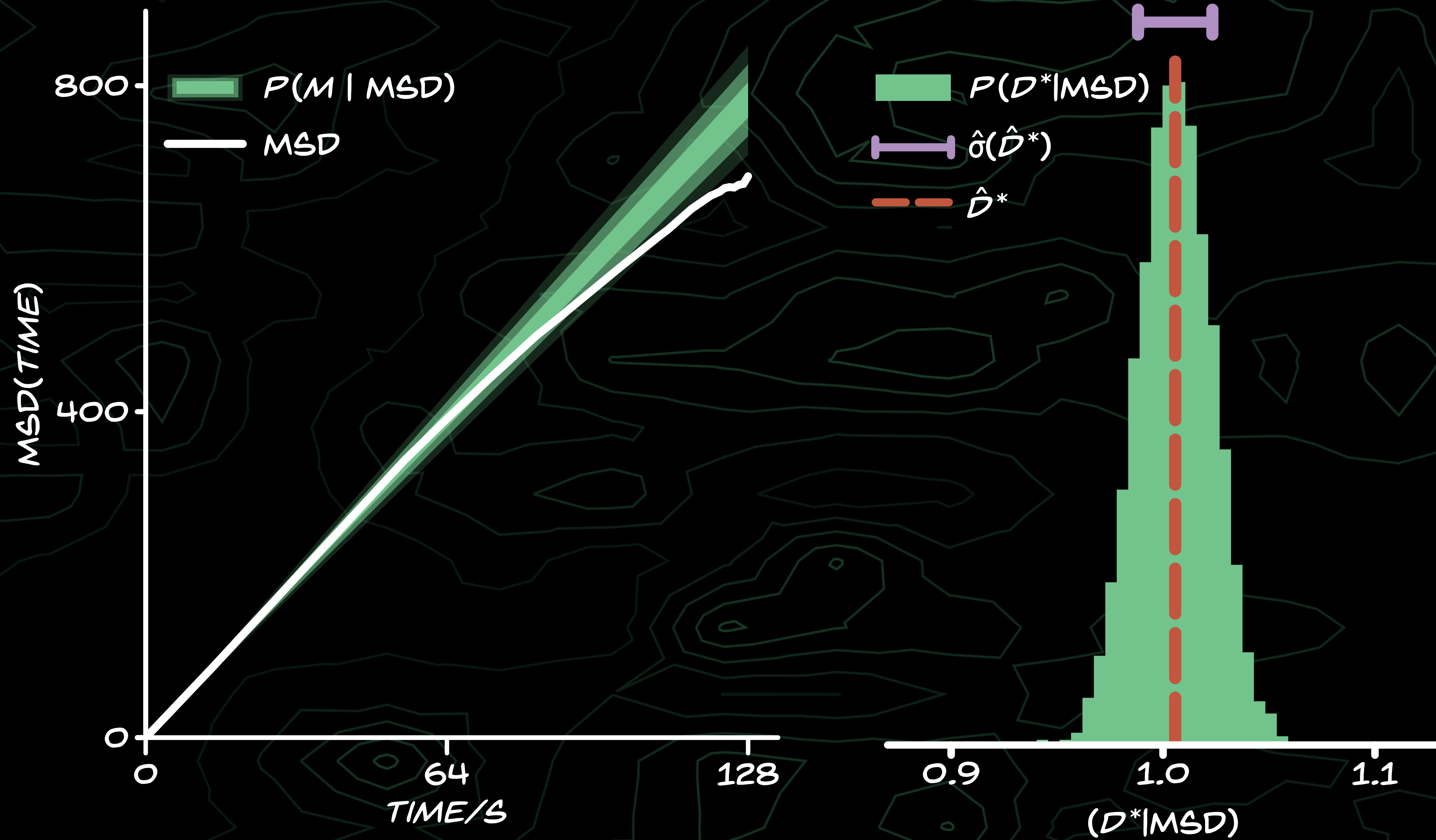


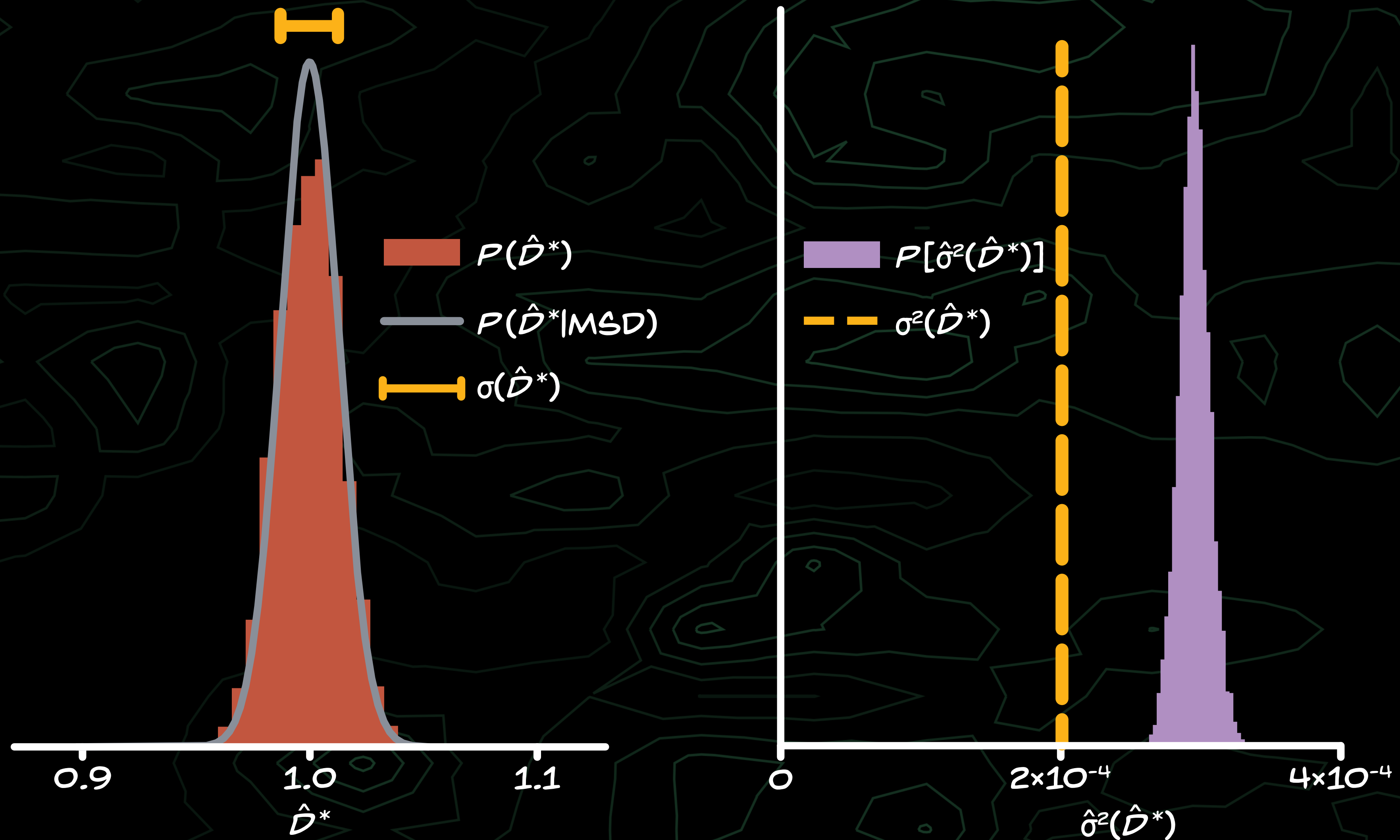
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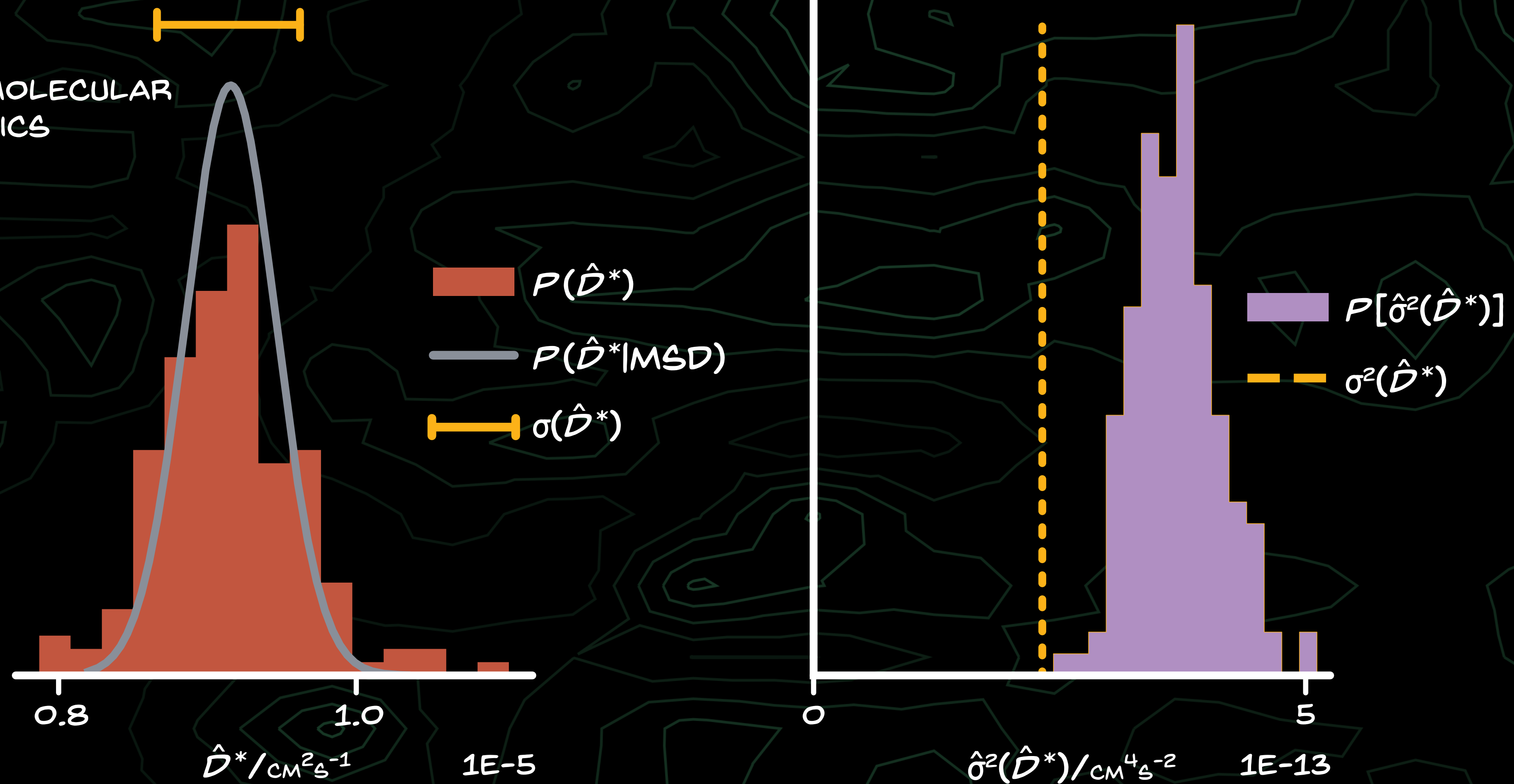
THE FULL COVARIANCE MATRIX CAN BE MODELLED BASED ON FREELY DIFFUSING PARTICLES.





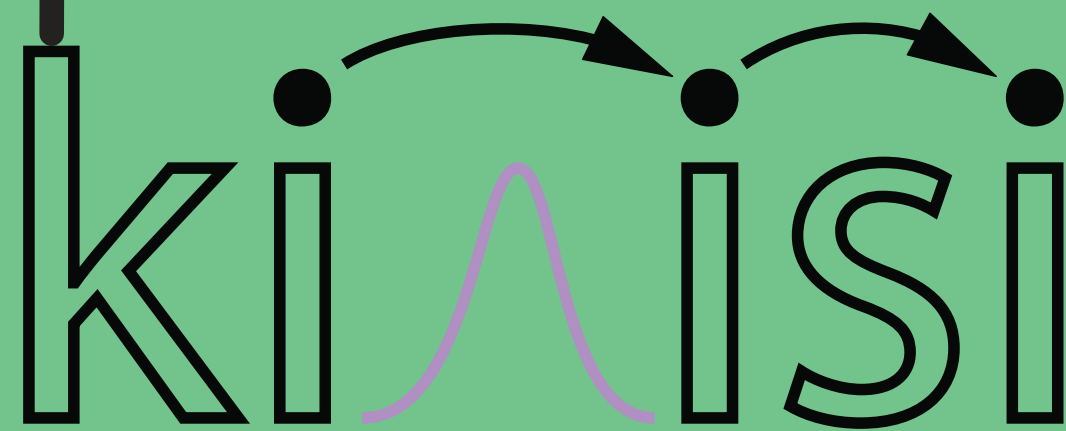


LLZO MOLECULAR DYNAMICS



**AVAILABLE NOW!
OPEN-SOURCE!**

WITH SUPPORT
FOR PYMATGEN, ASE,
AND MDANALYSIS
OBJECTS



`pip install kinisi`

KINISI.RTFD.IO



ARRHENIUS MODELLING CAN
BE USED FOR DIFFUSION...



...AND WITHOUT ERROR BARS
RESULTS ARE MEANINGLESS.



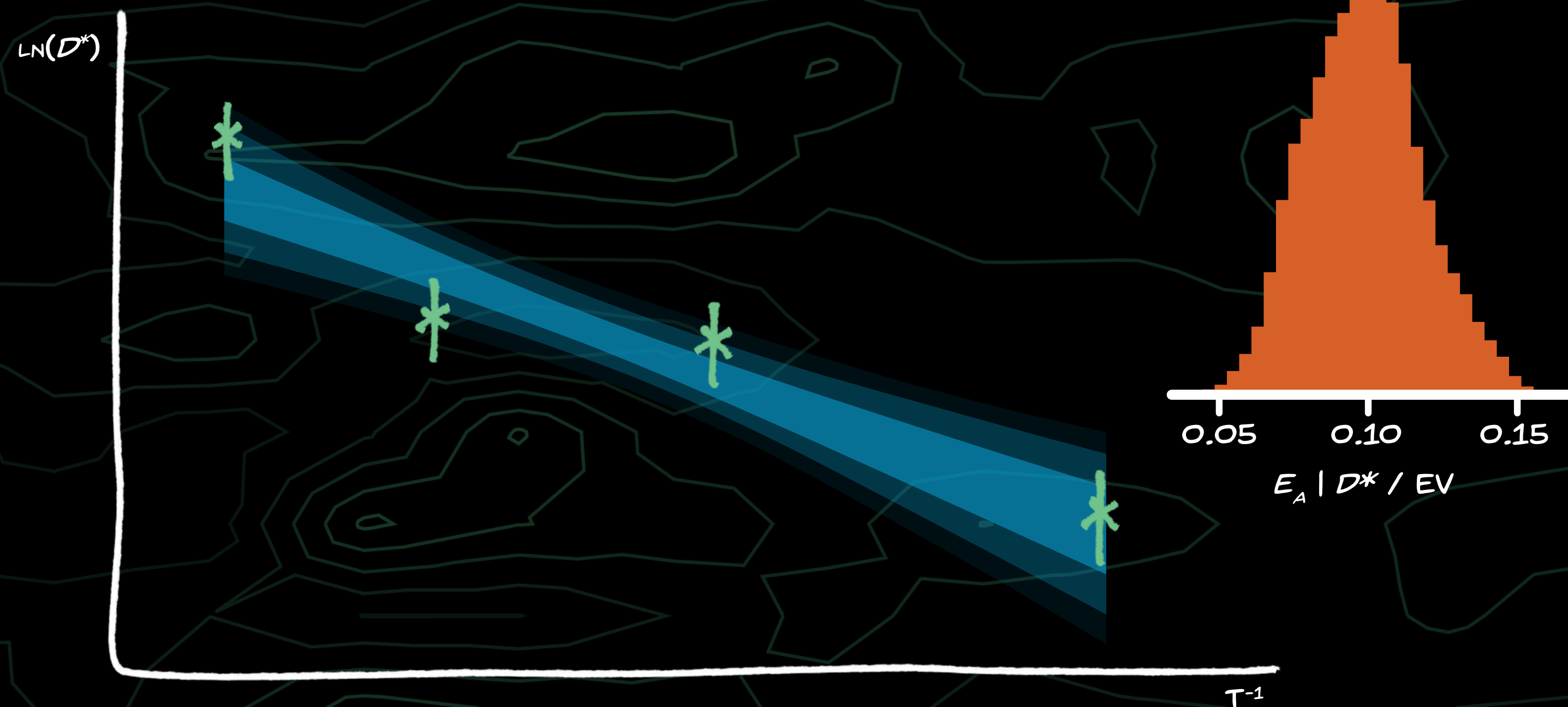
ARRHENIUS MODELLING CAN
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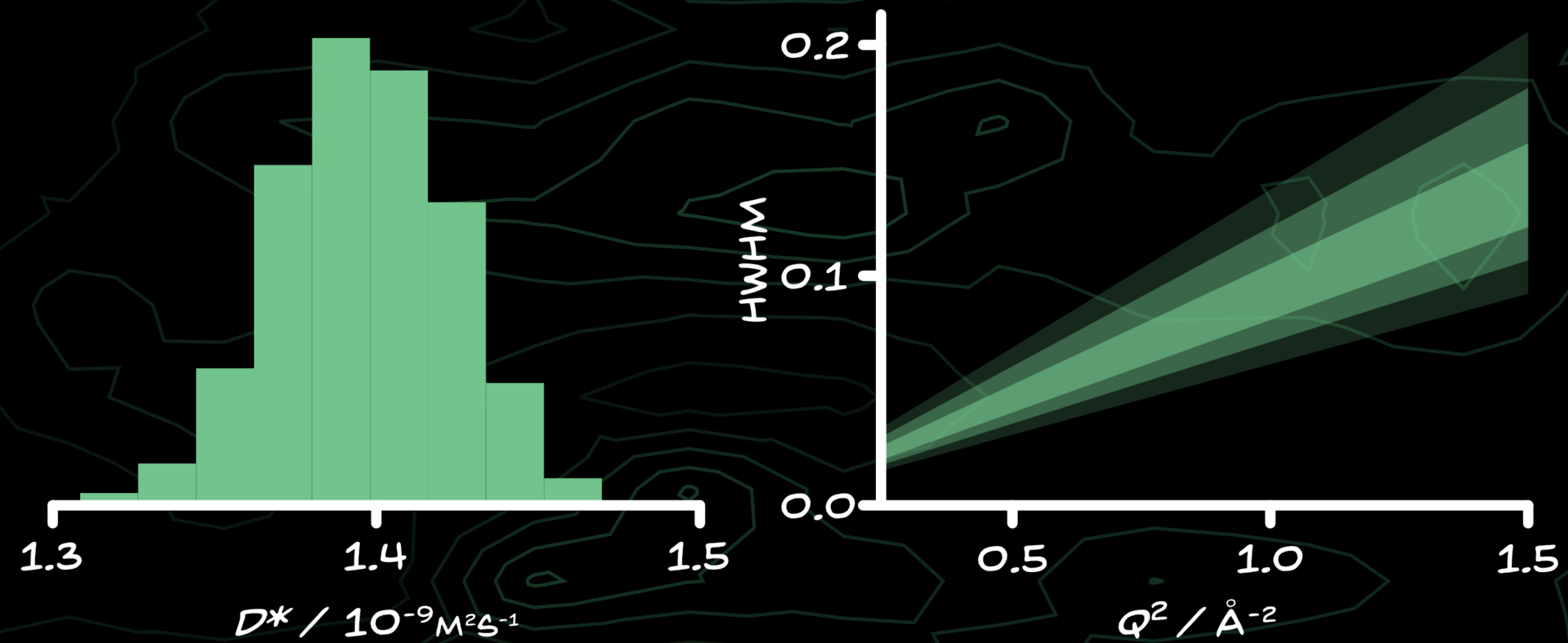
...AND WITHOUT ERROR BARS
RESULTS ARE MEANINGLESS.



WE CAN THEN PROPAGATE THE ERROR IN D^* TO THE ERROR IN THE
ACTIVATION ENERGY OF DIFFUSION.



WELL BUSTER, WE CAN USE PRIOR KNOWLEDGE FROM SIMULATION IN OUR QENS ANALYSIS.*



*THE PHD PROJECT OF HARRY RICHARDSON, WHO UNFORTUNATELY COULD NOT ATTEND.

ATOMS, IONS, OR MOLECULES
MIGHT PREFER TO MOVE IN
OPPOSITE DIRECTIONS...



...OR PERHAPS THEY DON'T
INTERACT....



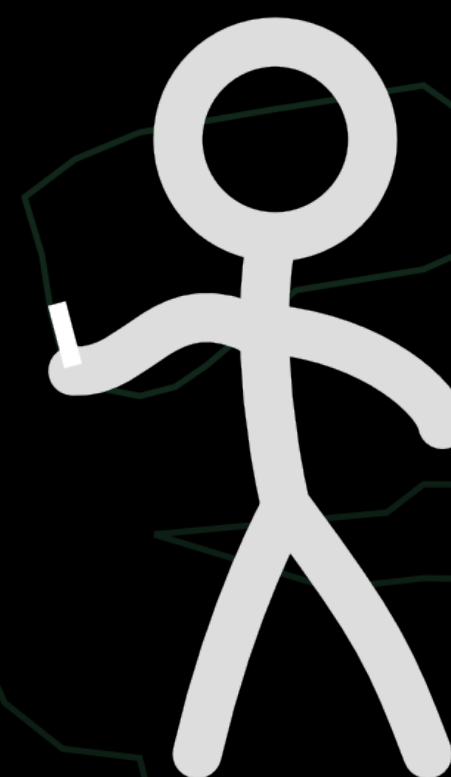
...OR THEY MAY SHOW COLLECTIVE
CONSTRUCTIVE MOTION.



The Nernst-Einstein Relation

albert
woz here

$$\sigma = \frac{Cq^2}{k_b T} D^*$$

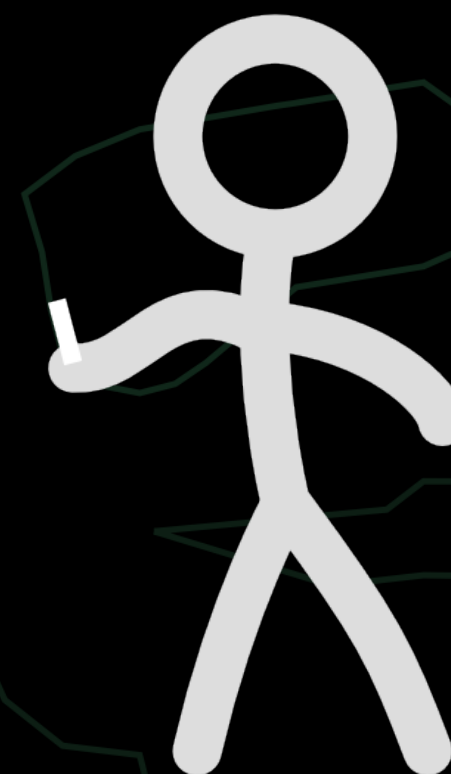


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The Nernst-Einstein Relation

albert
woz here

$$\sigma = \frac{Cq^2}{k_b T} D^*$$



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BRISTOL

The Nernst-Einstein Relation

$$\sigma = \frac{Cq^2}{k_b T} D^*$$

$$\sigma = \frac{Cq^2}{k_b T} \frac{D^*}{H_R}$$

albert
woz here

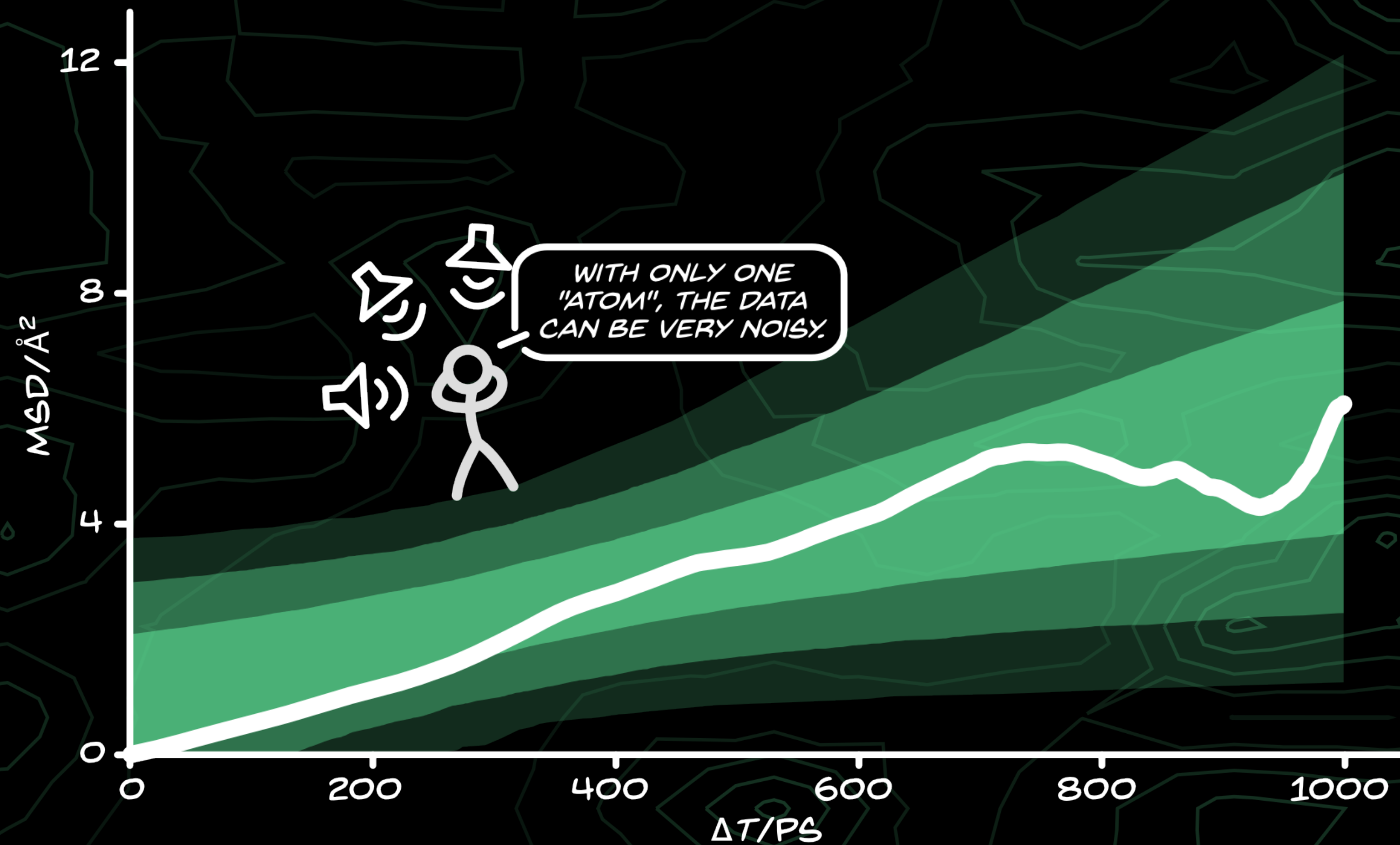
$$H_R = \frac{D^*}{D_0}$$

YOU SEE,
CORRELATION
IS IMPORTANT
TO UNDERSTAND
CONDUCTIVITY.

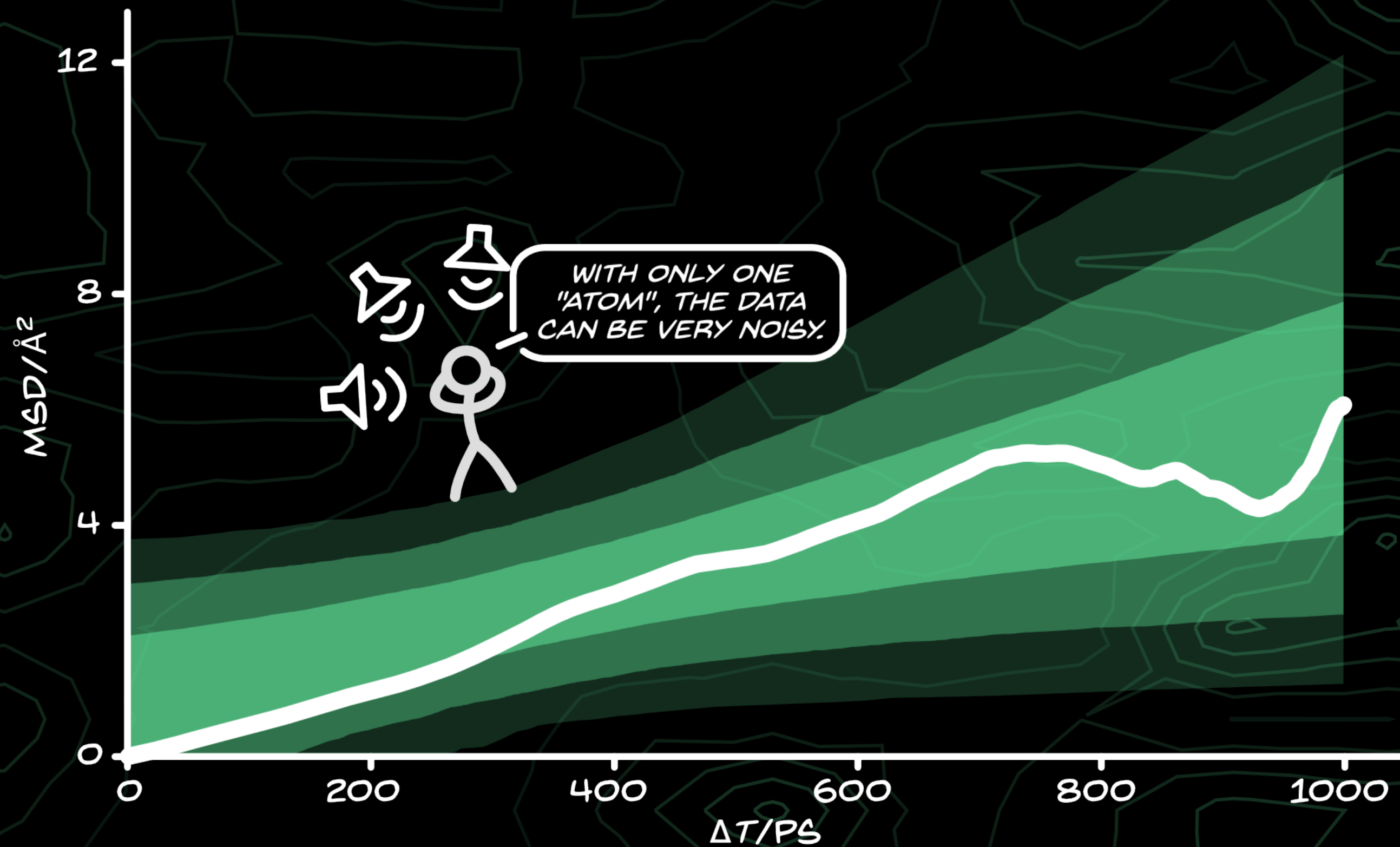


University of
BRISTOL

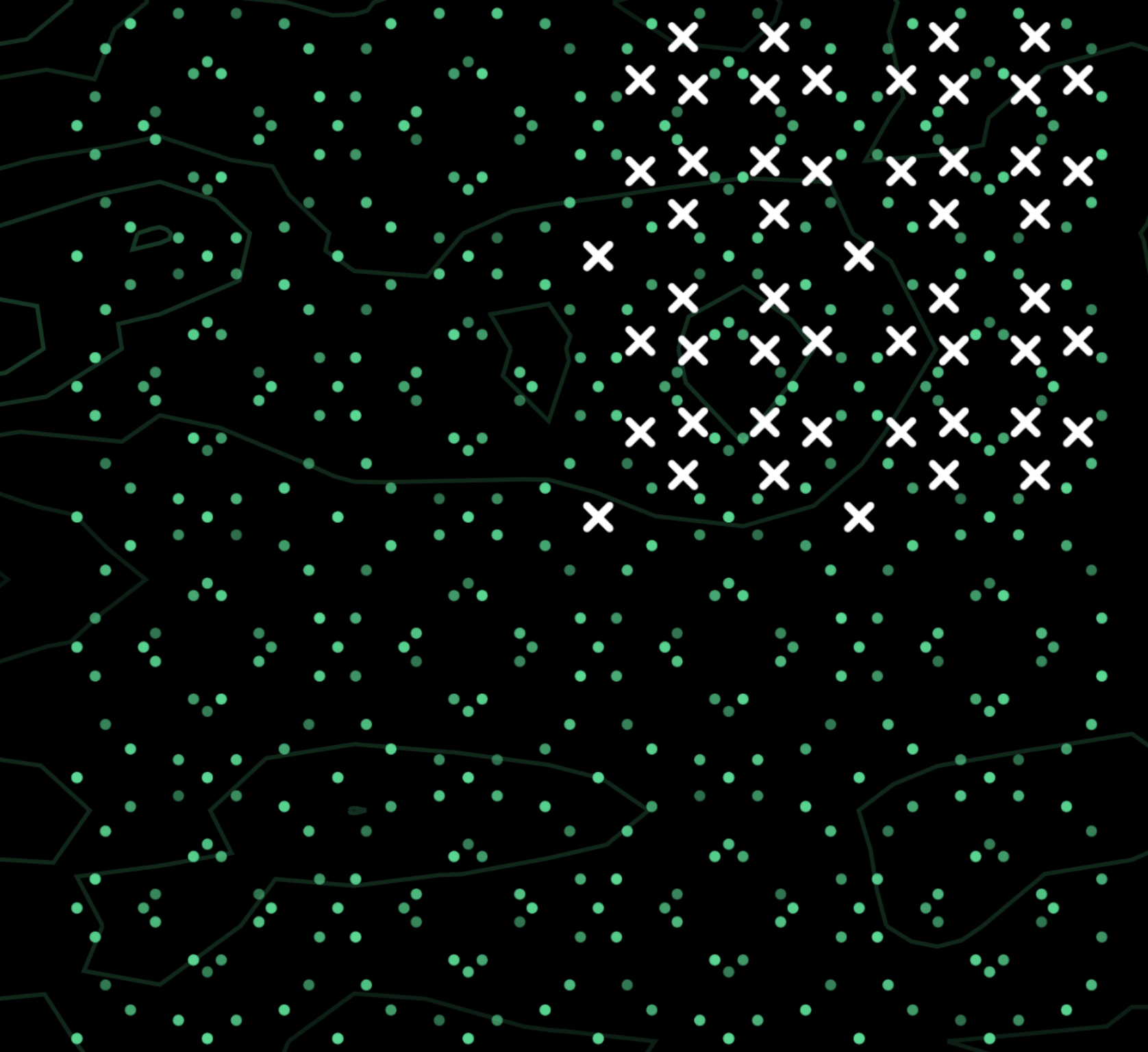
TO COMPUTE D_0 AND, THEREFORE H_R , WE NEED TO COMPUTE THE CENTRE-OF MASS MEAN-SQUARED DISPLACEMENT.



TO COMPUTE D_0 AND, THEREFORE H_R , WE NEED TO COMPUTE THE CENTRE-OF MASS MEAN-SQUARED DISPLACEMENT.

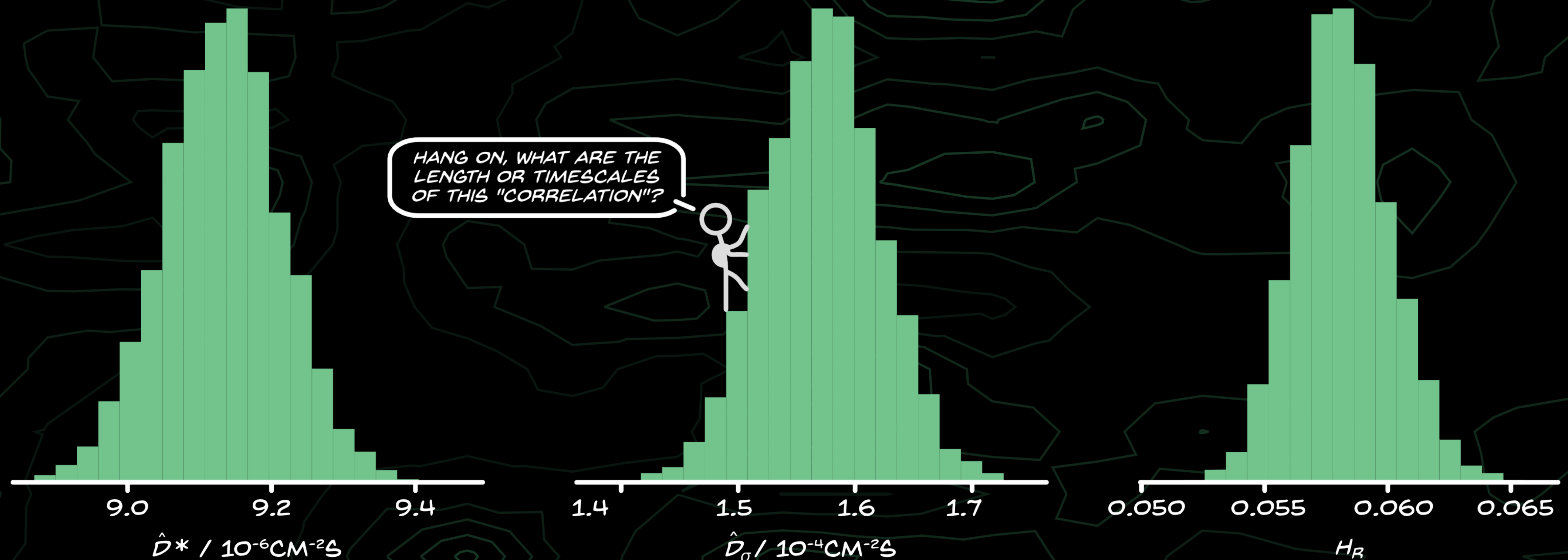


IF WE HAVE A BIG ENOUGH SIMULATION DATA, WE CAN DEFINE SUB CENTRES-OF-MASS.



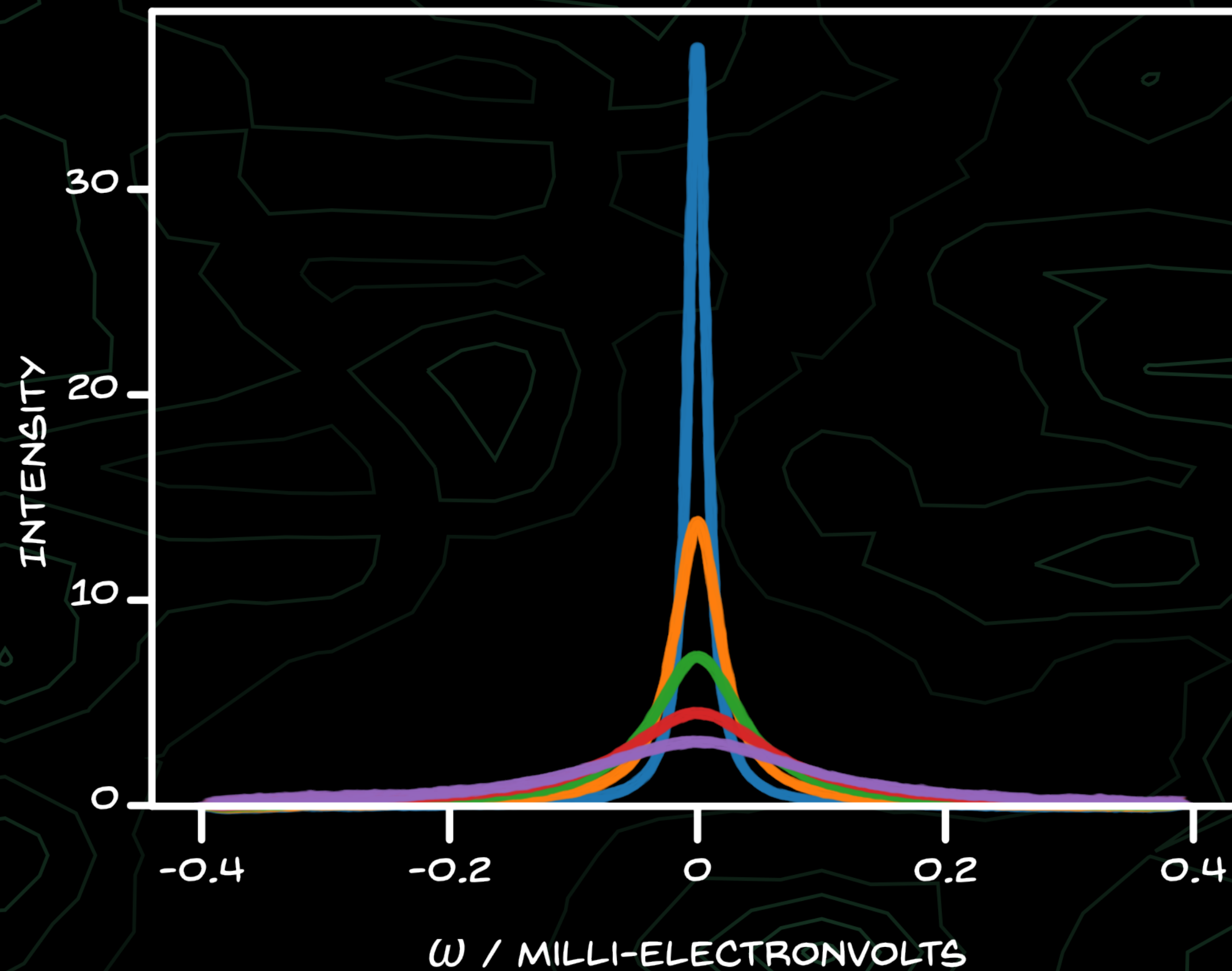
2 X 2 X 2 SUPERCELL LLZO (448 LITHIUM IONS)

WITH THIS APPROACH, WE CAN ESTIMATE THE HAVEN RATIO, AND, THEREFORE, THE AMOUNT OF CORRELATION IN OUR SYSTEM. IT LOOKS LIKE LLZO IS HIGHLY CORRELATED?*



*THIS IS VERY NEW DATA/CODE.

QENS IS AN EXCELLENT TOOL TO PROBE DIFFUSION...



...AND POLARISED-QENS PROVIDES AN
TOOL TO MEASURE THIS CORRELATION.

NEUTRON
MAN, HERE TO
SAVE THE DAY!



Ben Morgan (Bath)

Alexander Squires (Birmingham)

Samuel Coles (Bath/Cambridge)

Josh Dunn (Bristol)

Harry Richardson (Bristol)

Jeff Armstrong (ISIS)

Kit McColl (Bath)

*THANKS FOR
LISTENING!*

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scams-research.github.io

